AMOP Lecture 15
- Wed. 4.09 2014

Based on QTCA Lectures 24-25
Group Theory in Quantum Mechanics

Introduction to Rotational Eigenstates and Spectra I

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 7 Ch. 21-25)
(PSDS - Ch. 5, 7)

Review : *Applications of R(3) rotation and U(2) representations*
Molecular and nuclear wavefunctions
Molecular and nuclear eigenlevels
Example of CO_2 rovibration (υ=0)⇔(υ=1)bands
Generalized Stern-Gerlach and transformation matrices
Angular momentum cones and high J properties
Asymmetric Top eigensolutions for J=1-2
New geometric approach to rotational eigenstates and spectra

As of April 3, 2014

Links to the current Harter-Soft LearnIt web apps for Physics

Bold links have default redirect pages. ***Italics*** **are not yet meant for production.Red: the final stages of testing.**

List of *production* Harter-Soft Web Apps & Textbooks (For public)

Classical Mechanics with a Bang! - URL is "http://www.uark.edu/ua/modphys/markup/CMwBangWeb.html"
Quantum Theory for the Computer Age - URL is "http://www.uark.edu/ua/modphys/markup/QTCAWeb.html"
LearnIt Web Applications - URL is "http://www.uark.edu/ua/modphys/markup/LearnItWeb.html"

Individual web-apps for current classes:

BohrIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BohrItWeb.html"
BounceIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BounceItWeb.html"
BoxIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BoxItWeb.html"
CoulIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/CoulItWeb.html"
Cycloidulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html"
JerkIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/JerkItWeb.html"
MolVibes - Production; URL is "http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html"
Pendulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/PendulumWeb.html"
QuantIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"

The old relativity website (2005):
Relativity - Pirelli Entrant - Production; URL is "**http://www.uark.edu/ua/pirelli**" or "http://www.uark.edu/ua/pirelli/html/default.html"

Newer relativity web-apps currently being developed (2013-)
RelativIt Production; URL is "http://www.uark.edu/ua/modphys/markup/RelativItWeb.html"
RelaWavity Production; URL is "http://www.uark.edu/ua/modphys/markup/RelaWavityWeb.html"

Additional classical wep-apps:
Trebuchet Production; URL is "http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html"
WaveIt Production; URL is "http://www.uark.edu/ua/modphys/markup/WaveItWeb.html"

Link to master list of all Harter-Soft Web Apps & Textbooks (Prod, Testing, & Developement)

http://www.uark.edu/ua/modphys/testing/markup/Harter-SoftWebApps.html

Generating R(3) rotation and U(2) representations

Applications of R(3) rotation and U(2) representations

Molecular and nuclear wavefunctions

Molecular and nuclear eigenlevels

Example of CO_2 rovibration $(\upsilon=0)\Leftrightarrow(\upsilon=1)$bands

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high J properties

Applications of R(3) rotation and U(2) representations

Vector ($j=\ell=1$) representation

$$D^1(\alpha\beta\gamma)=\begin{pmatrix} e^{-i\alpha} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\alpha}\end{pmatrix}\begin{pmatrix} \frac{1+\cos\beta}{2} & \frac{-\sin\beta}{\sqrt{2}} & \frac{1-\cos\beta}{2} \\ \frac{\sin\beta}{\sqrt{2}} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}} \\ \frac{1-\cos\beta}{2} & \frac{\sin\beta}{\sqrt{2}} & \frac{1+\cos\beta}{2}\end{pmatrix}\begin{pmatrix} e^{-i\gamma} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{i\gamma}\end{pmatrix}=\begin{pmatrix} e^{-i\alpha}\frac{1+\cos\beta}{2}e^{-i\gamma} & e^{-i\alpha}\frac{-\sin\beta}{\sqrt{2}} & e^{-i\alpha}\frac{1-\cos\beta}{2}e^{i\gamma} \\ \frac{\sin\beta}{\sqrt{2}}e^{-i\gamma} & \cos\beta & \frac{-\sin\beta}{\sqrt{2}}e^{i\gamma} \\ e^{i\alpha}\frac{1-\cos\beta}{2}e^{-i\gamma} & e^{i\alpha}\frac{\sin\beta}{\sqrt{2}} & e^{i\alpha}\frac{1+\cos\beta}{2}e^{i\gamma}\end{pmatrix}$$

Here half-angle identities were used. $\cos^2\frac{\beta}{2}=\frac{1+\cos\beta}{2}$, $\sin^2\frac{\beta}{2}=\frac{1-\cos\beta}{2}$, $\sin\frac{\beta}{2}\cos\frac{\beta}{2}=\frac{\sin\beta}{2}$,

$$Y_1^1(\phi,\theta)=\sqrt{\tfrac{3}{4\pi}}e^{-i\phi}\frac{-\sin\theta}{\sqrt{2}}$$

$$Y_0^1(\phi,\theta)=\sqrt{\tfrac{3}{4\pi}}\cos\beta$$

$$Y_{-1}^1(\phi,\theta)=\sqrt{\tfrac{3}{4\pi}}e^{+i\phi}\frac{\sin\theta}{\sqrt{2}}$$

Center ($n=0$) column with the factor $\sqrt{\frac{2\ell+1}{4\pi}}$ gives set of *spherical harmonics* Y^ℓ_m.

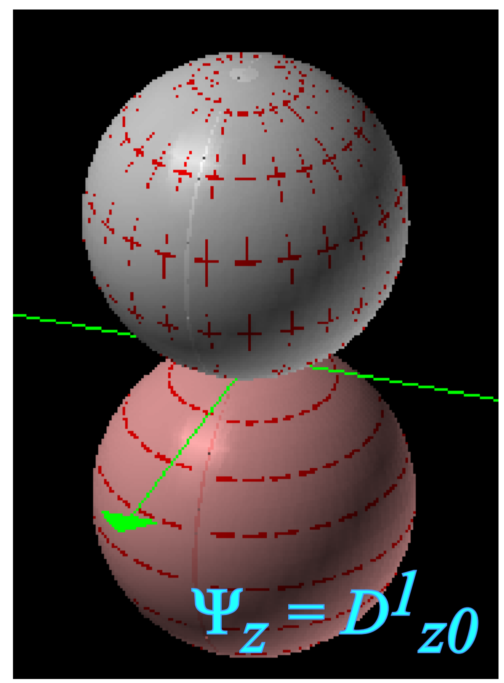
$$Y^\ell_m(\phi\theta)=D^{\ell*}_{m,n=0}(\phi\theta 0)\sqrt{\frac{2\ell+1}{4\pi}}$$

Dipole ($j=\ell=1$) waves

$$D^{1*}_{1,0}(\phi\theta 0)=-e^{i\phi}\frac{\sin\theta}{\sqrt{2}}=-\frac{\cos\phi\sin\theta+i\cos\phi\sin\theta}{\sqrt{2}}=-\frac{x+iy}{r\sqrt{2}}$$

$$D^{1*}_{0,0}(\phi\theta 0)=\cos\theta=\cos\theta=z/r$$

$$D^{1*}_{-1,0}(\phi\theta 0)=e^{-i\phi}\frac{\sin\theta}{\sqrt{2}}=\frac{\cos\phi\sin\theta-i\cos\phi\sin\theta}{\sqrt{2}}=\frac{x-iy}{r\sqrt{2}}$$

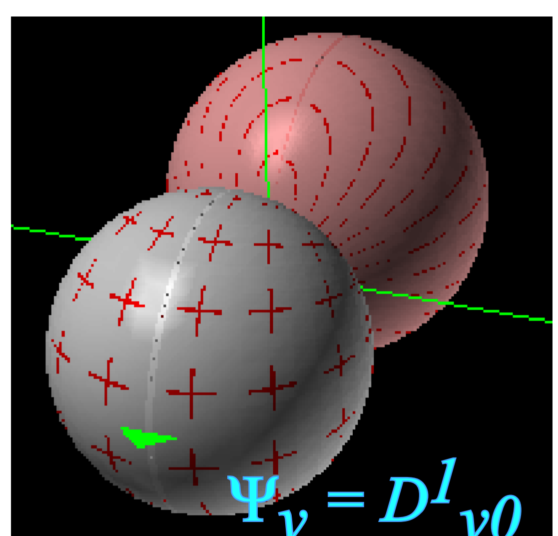


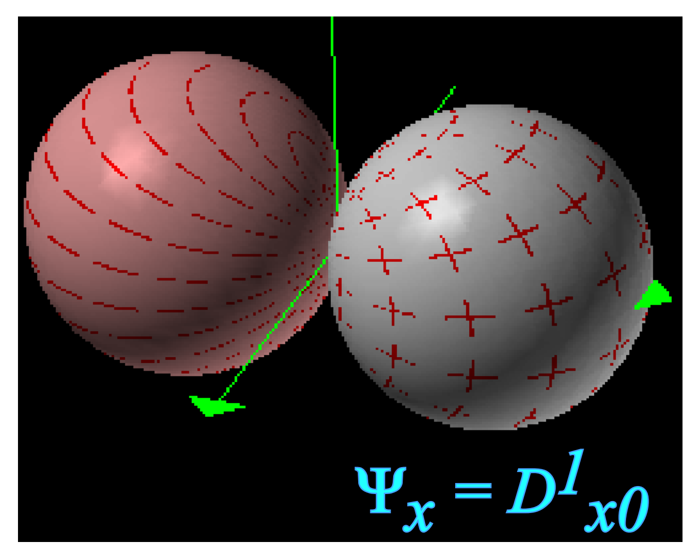
j = 1
Standing
p-Waves

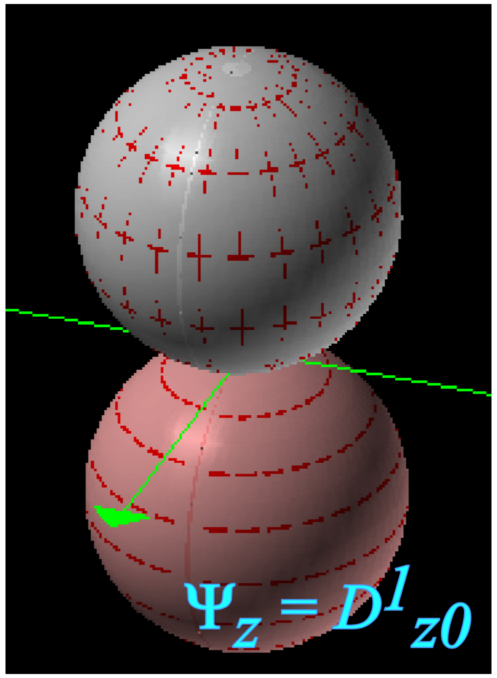
$$\Psi^1_x(\phi,\theta)=D^1_{x,z}(\phi,\theta,0)=\cos\phi\sin\theta$$

$$\Psi^1_y(\phi,\theta)=D^1_{y,z}(\phi,\theta,0)=\sin\phi\sin\theta$$

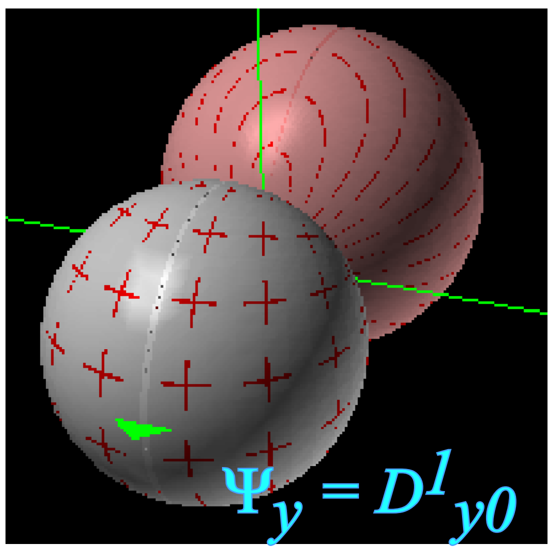
$$\Psi^1_z(\phi,\theta)=D^1_{z,z}(\phi,\theta,0)=\cos\theta$$

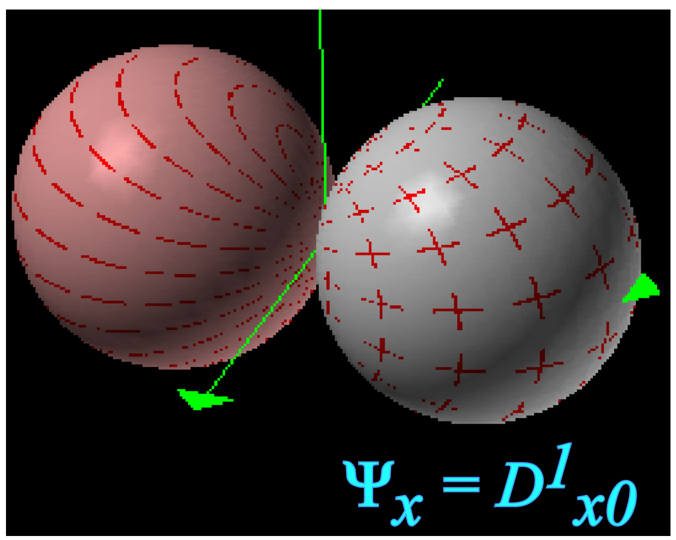






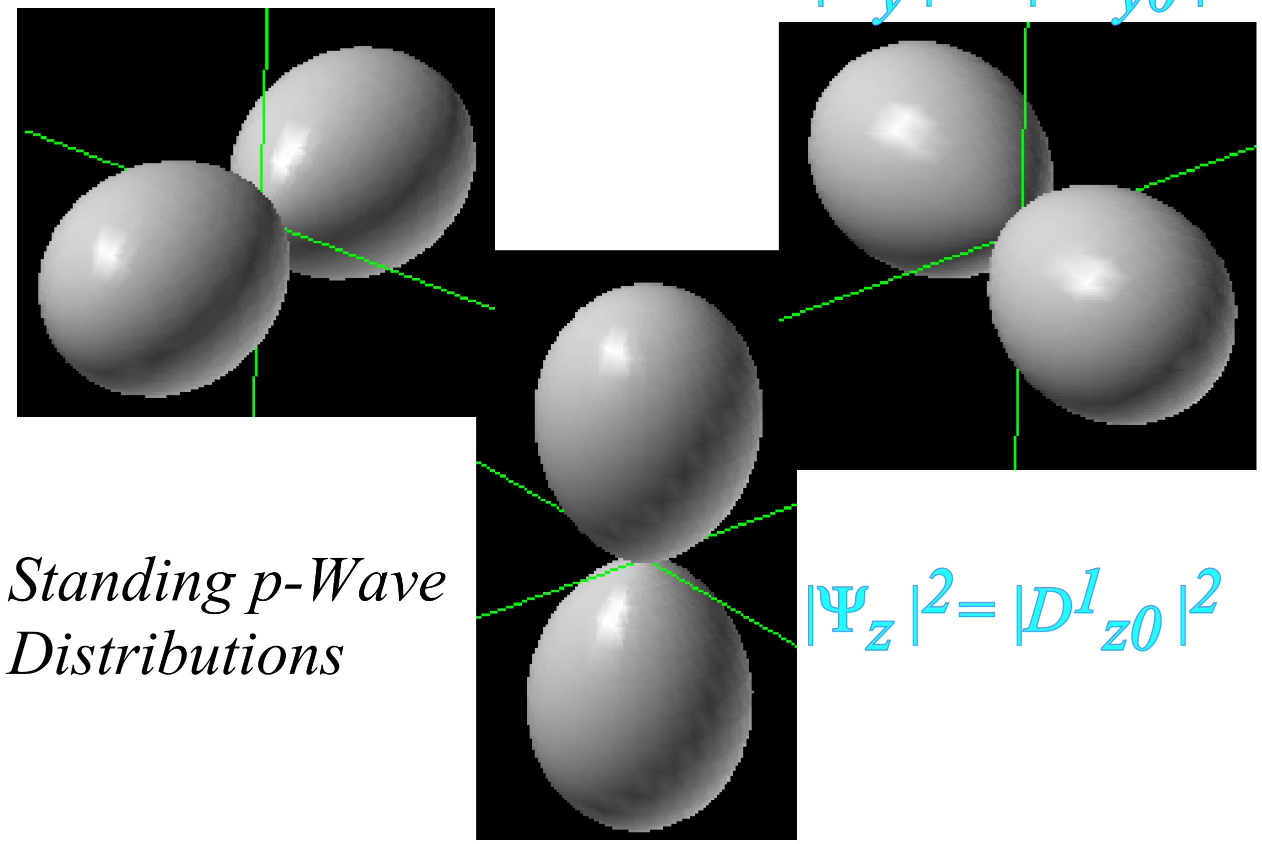
j = 1
Standing
p-Waves





$$\Psi^1_x(\phi,\theta) = D^1_{x,z}(\phi,\theta,0)$$
$$= \cos\phi\sin\theta$$
$$\Psi^1_y(\phi,\theta) = D^1_{y,z}(\phi,\theta,0)$$
$$= \sin\phi\sin\theta$$
$$\Psi^1_z(\phi,\theta) = D^1_{z,z}(\phi,\theta,0)$$
$$= \cos\theta$$

$|\Psi_x|^2 = |D^1{}_{x0}|^2$ $|\Psi_y|^2 = |D^1{}_{y0}|^2$

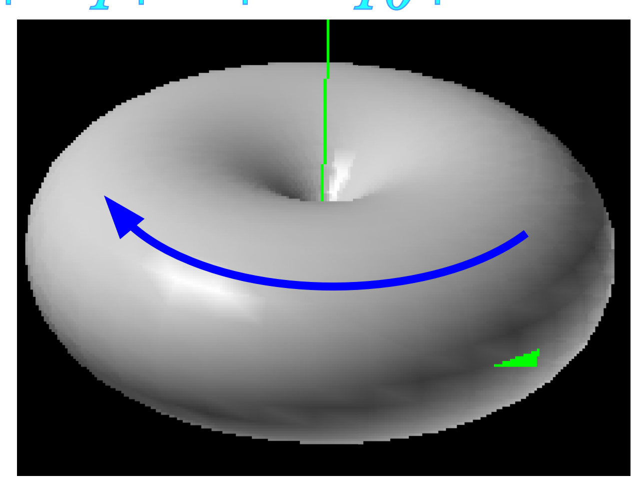


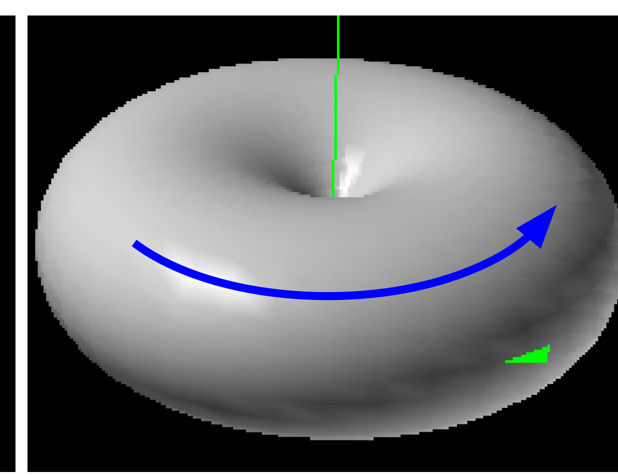
Standing p-Wave Distributions

$|\Psi_z|^2 = |D^1{}_{z0}|^2$

Moving p-Wave Distributions

$|\Psi_{-1}|^2 = |D^1{}_{-10}|^2$ $|\Psi_1|^2 = |D^1{}_{10}|^2$





Applications of R(3) rotation and U(2) representations

Tensor (j=ℓ=2) representation

$$D^2(\alpha\beta 0)=\left(\begin{array}{cc|c|cc}
e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\
e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\
\sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\
e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\
e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2
\end{array}\right)$$

Applications of R(3) rotation and U(2) representations

Tensor (j=ℓ=2) representation

$$D^2(\alpha\beta 0)=\left(\begin{array}{cc|c|cc}
e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\
e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\
\sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\
e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\
e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2
\end{array}\right)$$

Spherical 2^k-*multipole functions* $X^k{}_q$ or *X-functions* are D^*-functions times the k^{th} power of radius (r^k).

$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=2}(\phi\theta)=D^{2*}_{2,0}(\phi\theta 0)=\sqrt{\frac{3}{8}}e^{i2\phi}\sin^2\theta=\sqrt{\frac{3}{8}}\frac{(x+iy)^2}{r^2}$$

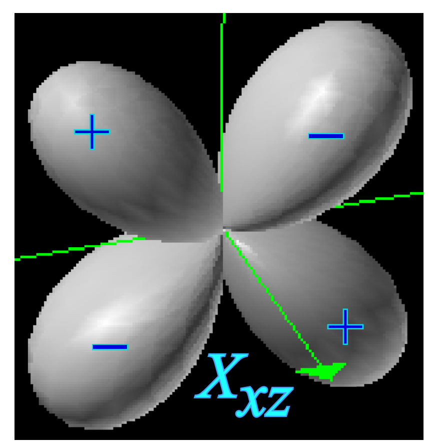
$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=1}(\phi\theta)=D^{2*}_{1,0}(\phi\theta 0)=-\sqrt{\frac{3}{2}}e^{i\phi}\sin\theta\cos\theta=-\sqrt{\frac{3}{2}}\frac{(x+iy)z}{r^2}$$

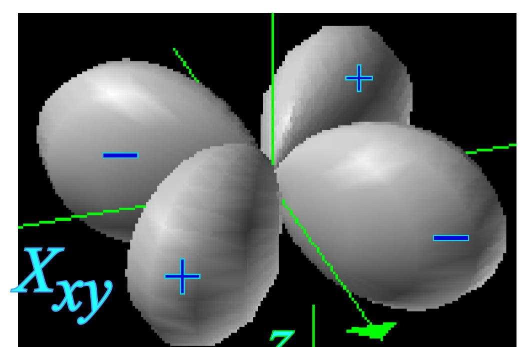
$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=0}(\phi\theta)=D^{2*}_{0,0}(\phi\theta 0)=\frac{3\cos^2\theta-1}{2}=\frac{3z^2-r^2}{2r^2}$$

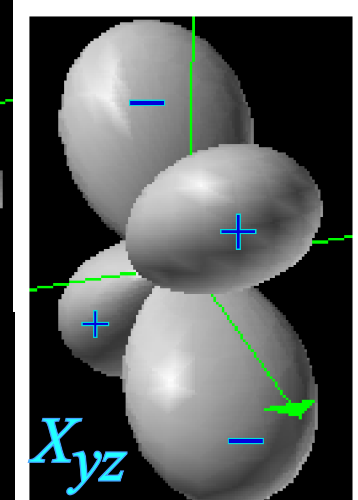
$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=-1}(\phi\theta)=D^{2*}_{-1,0}(\phi\theta 0)=\sqrt{\frac{3}{2}}e^{-i\phi}\sin\theta\cos\theta=\sqrt{\frac{3}{2}}\frac{(x-iy)z}{r^2}$$

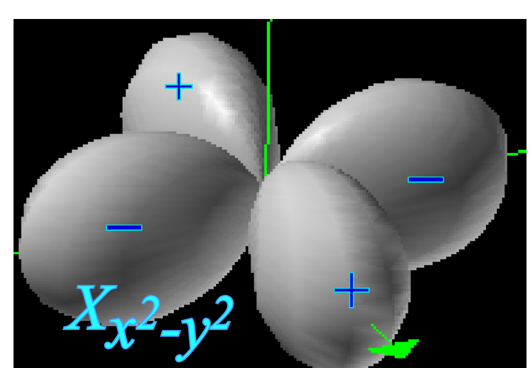
$$\sqrt{4\pi/5}\,Y^{\ell=2}_{m=-2}(\phi\theta)=D^{2*}_{-2,0}(\phi\theta 0)=\sqrt{\frac{3}{8}}e^{-i2\phi}\sin^2\theta=\sqrt{\frac{3}{8}}\frac{(x-iy)^2}{r^2}$$

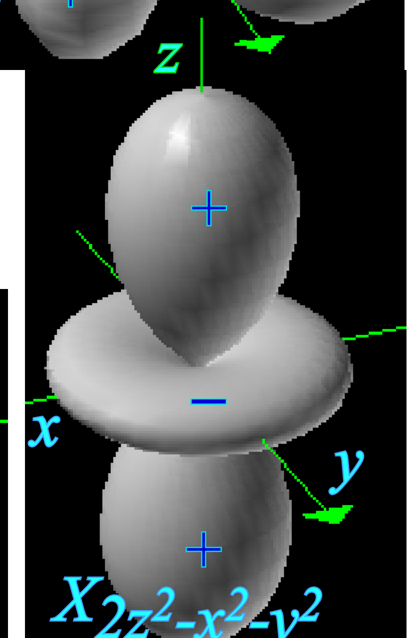
$$X^k_q=r^kD^{k*}_{q,0}=\sqrt{\frac{4\pi}{2k+1}}r^kY^k_q$$











j = 2
Standing d-Waves

Tensor (j=ℓ=2) representation

Spherical 2^k*-multipole functions* $X^k{}_q$ or *X-functions* are D^*-functions times the k^{th} power of radius (r^k).

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=2}(\phi\theta) = D^{2*}_{2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}} e^{i2\phi}\sin^2\theta = \sqrt{\frac{3}{8}}\frac{(x+iy)^2}{r^2}$$

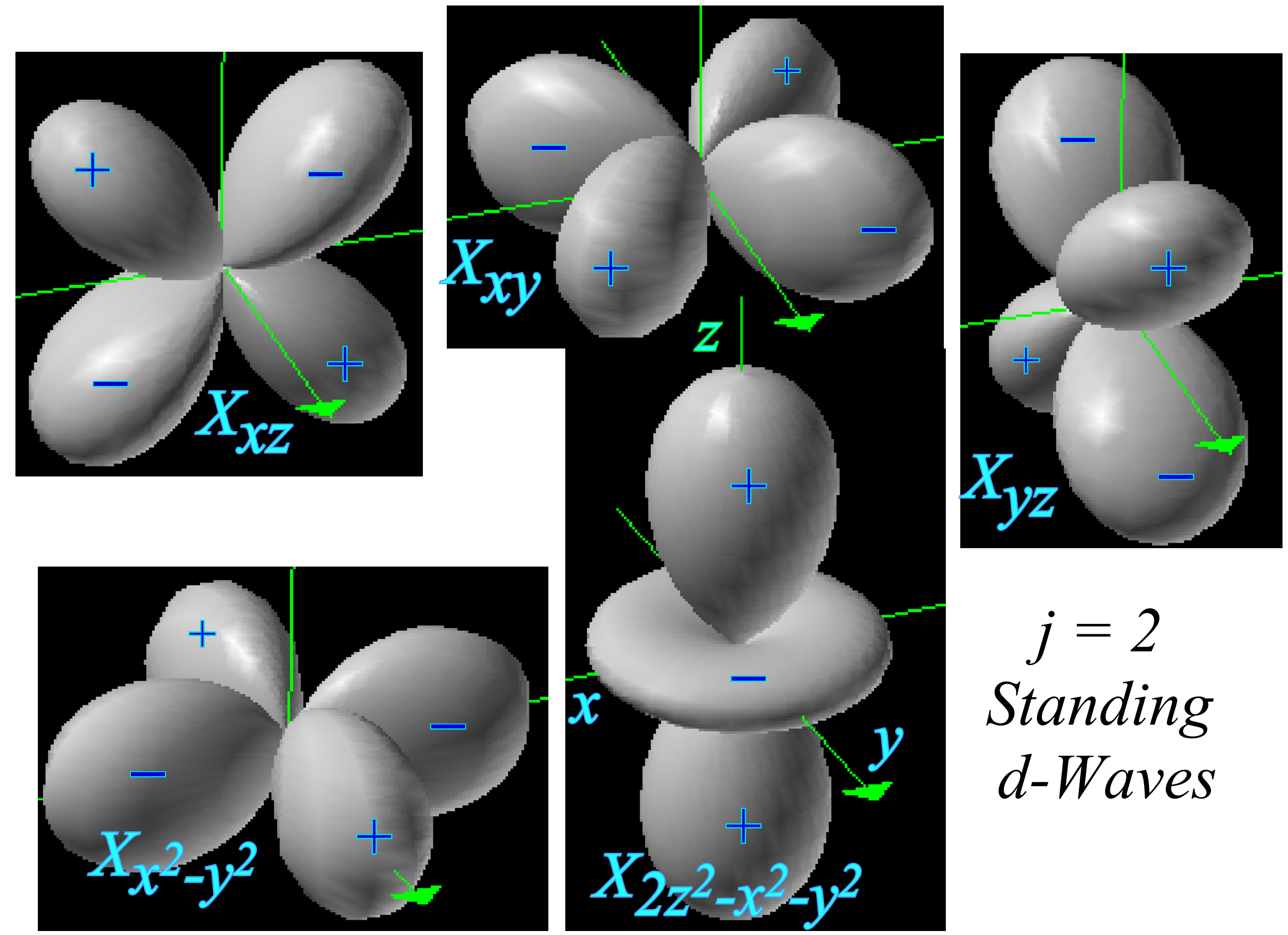
$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=1}(\phi\theta) = D^{2*}_{1,0}(\phi\theta 0) = -\sqrt{\frac{3}{2}} e^{i\phi}\sin\theta\cos\theta = -\sqrt{\frac{3}{2}}\frac{(x+iy)z}{r^2}$$

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=0}(\phi\theta) = D^{2*}_{0,0}(\phi\theta 0) = \frac{3\cos^2\theta - 1}{2} = \frac{3z^2 - r^2}{2r^2}$$

$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=-1}(\phi\theta) = D^{2*}_{-1,0}(\phi\theta 0) = \sqrt{\frac{3}{2}} e^{-i\phi}\sin\theta\cos\theta = \sqrt{\frac{3}{2}}\frac{(x-iy)z}{r^2}$$

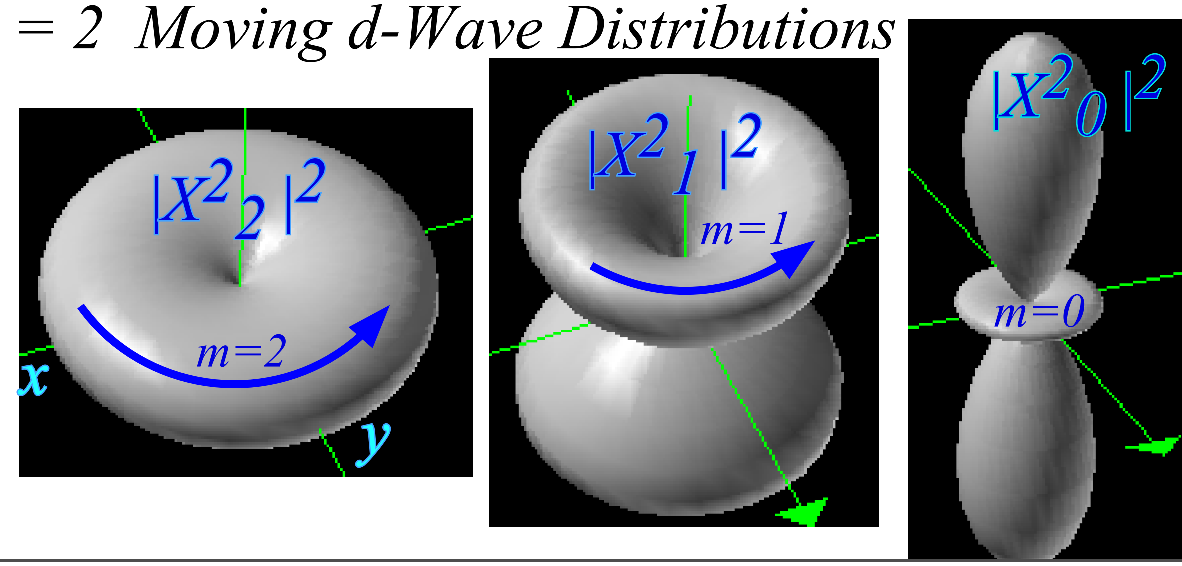
$$\sqrt{4\pi/5}\, Y^{\ell=2}_{m=-2}(\phi\theta) = D^{2*}_{-2,0}(\phi\theta 0) = \sqrt{\frac{3}{8}} e^{-i2\phi}\sin^2\theta = \sqrt{\frac{3}{8}}\frac{(x-iy)^2}{r^2}$$

$$X^k_q = r^k D^{k*}_{q,0} = \sqrt{\frac{4\pi}{2k+1}}\, r^k Y^k_q$$



j = 2 Standing d-Waves

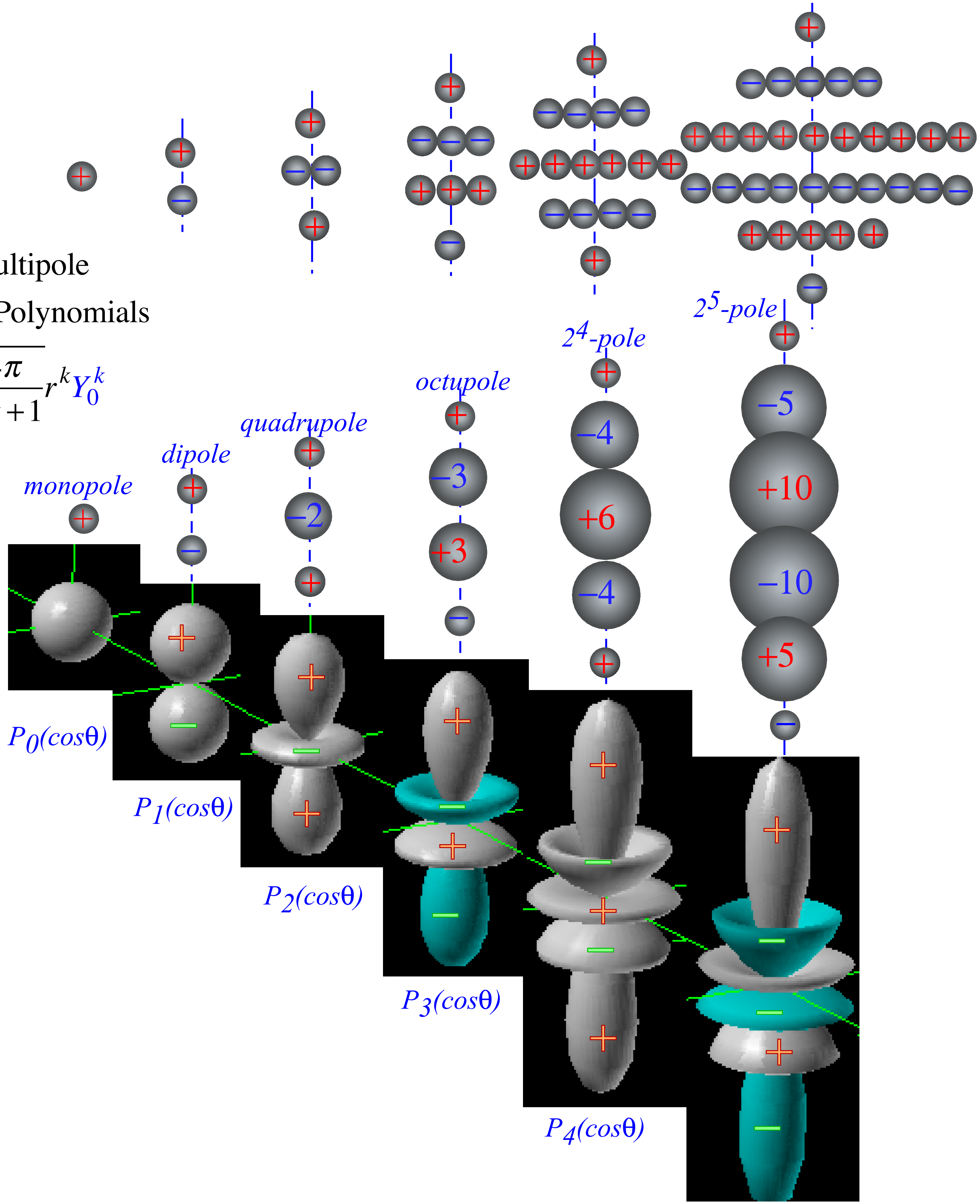
j = 2 Moving d-Wave Distributions



Legendre $P_k(\Theta)$ Multipole

Symmetric ($q=0$) Polynomials

$$X_0^k = r^k D_{0,0}^{k*} = \sqrt{\frac{4\pi}{2k+1}}\, r^k Y_0^k$$



Review :

Applications of R(3) rotation and U(2) representations

➡ *Molecular and nuclear wavefunctions* ⬅

Molecular and nuclear eigenlevels

Example of CO_2 rovibration $(\upsilon=0)\Leftrightarrow(\upsilon=1)$bands

Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high J properties

Applications of R(3) rotation and U(2) representations

Molecular and nuclear wavefunctions

For *SU(2)* and *R(3)*, sum over rotations is an integral over Euler angles *(αβγ)*.

For integral-*j=0, 1, 2,..* the *R(3)* integral over polar angle β ranges from 0 to π.

$$\text{for } R(3): \frac{\ell^j}{N}\int d(\alpha\beta\gamma) = \frac{2j+1}{8\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma \;= 2j+1 = \ell^j$$

For integral-*j=1/2, 3/2,..* the *U(2)* integral over polar angle β ranges from -π to π.

$$\text{for } SU(2): \frac{\ell^j}{N}\int d(\alpha\beta\gamma) = \frac{2j+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_{-\pi}^{\pi} d\beta \sin\beta \int_0^{2\pi} d\gamma \;= 2j+1 = \ell^j$$

Eigenstates of angular momentum are built from projected initial position states |000⟩.

$$\left|{}^{j}_{m,n}\right\rangle = \frac{\mathbf{P}^j_{m,n}|000\rangle}{\sqrt{\ell^j}} = \frac{1}{N}\int d(\alpha\beta\gamma)\,D^{j*}_{m,n}(\alpha\beta\gamma)\mathbf{R}(\alpha\beta\gamma)|000\rangle\sqrt{\ell^j} = \frac{1}{N}\int d(\alpha\beta\gamma)\,D^{j*}_{m,n}(\alpha\beta\gamma)\sqrt{\ell^j}\,|\alpha\beta\gamma\rangle$$

Angular position is defined by a *rotational duality relativity relation* or “Mock-Mach” principle

$$\mathbf{R}(\alpha\beta\gamma)|000\rangle = |\alpha\beta\gamma\rangle = \bar{\mathbf{R}}^\dagger(\alpha\beta\gamma)|000\rangle$$

$$\mathbf{R}(\alpha\beta\gamma)\bar{\mathbf{R}}(\alpha'\beta'\gamma') = \bar{\mathbf{R}}(\alpha'\beta'\gamma')\mathbf{R}(\alpha\beta\gamma)$$

$$\text{for all}(\alpha\beta\gamma)\text{and}(\alpha'\beta'\gamma')$$

Left hand (lab-*m*) and right hand (body-*n*) quantum numbers apply.

$$\mathbf{R}(\alpha\beta\gamma)\left|{}^{j}_{m,n}\right\rangle = \sum_{m'=-j}^{j} D^{j}_{m',m}(\alpha\beta\gamma)\left|{}^{j}_{m',n}\right\rangle \qquad \bar{\mathbf{R}}(\alpha\beta\gamma)\left|{}^{j}_{m,n}\right\rangle = \sum_{n'=-j}^{j} D^{j*}_{n',n}(\alpha\beta\gamma)\left|{}^{j}_{m,n'}\right\rangle$$

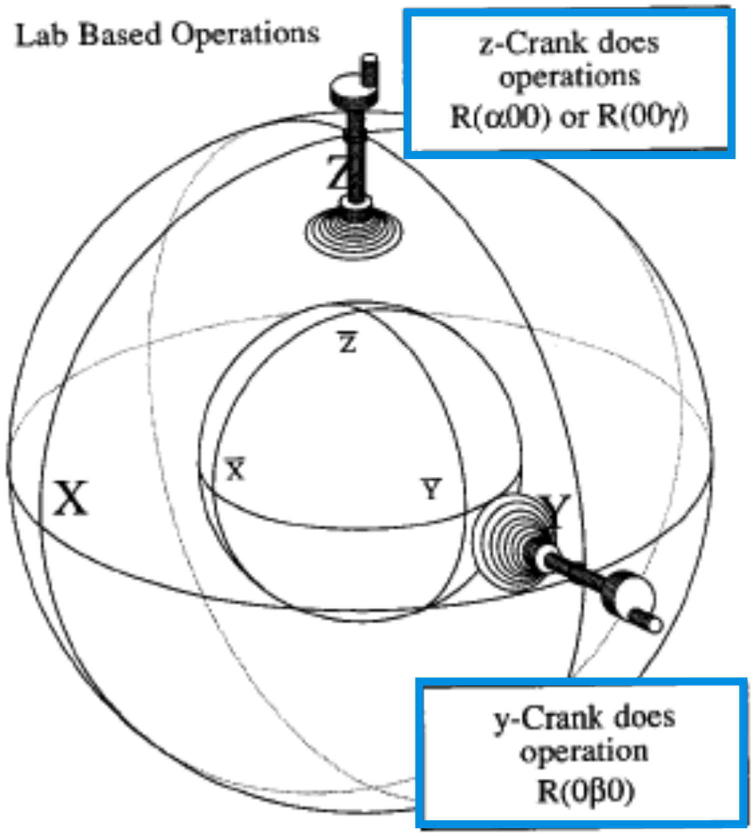
Same applies to the generators $\mathbf{s}_Z$ or $\mathbf{J}_Z$ of *SU(2)* or *R(3)*.

$$\mathbf{s}_Z\left|{}^{j}_{m,n}\right\rangle = m\left|{}^{j}_{m,n}\right\rangle \qquad \bar{\mathbf{s}}_Z\left|{}^{j}_{m,n}\right\rangle = -n\left|{}^{j}_{m,n}\right\rangle$$

"Give me a place to stand...
and I will move the Earth"
Archimedes 287-212 B.C.E

Ideas of duality/relativity go *way* back (...VanVleck, Casimir..., Mach, Newton, Archimedes...)

Lab-fixed(Extrinsic-Global)**R**,**S**,..*vs.* Body-fixed (Intrinsic-Local)$\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..



all **R**,**S**,..
commute with
all $\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..

"Mock-Mach"
relativity principles

$$\mathbf{R}|1\rangle=\bar{\mathbf{R}}^{-1}|1\rangle$$
$$\mathbf{S}|1\rangle=\bar{\mathbf{S}}^{-1}|1\rangle$$
$$\vdots$$

...for *one* state $|1\rangle$ *only!*

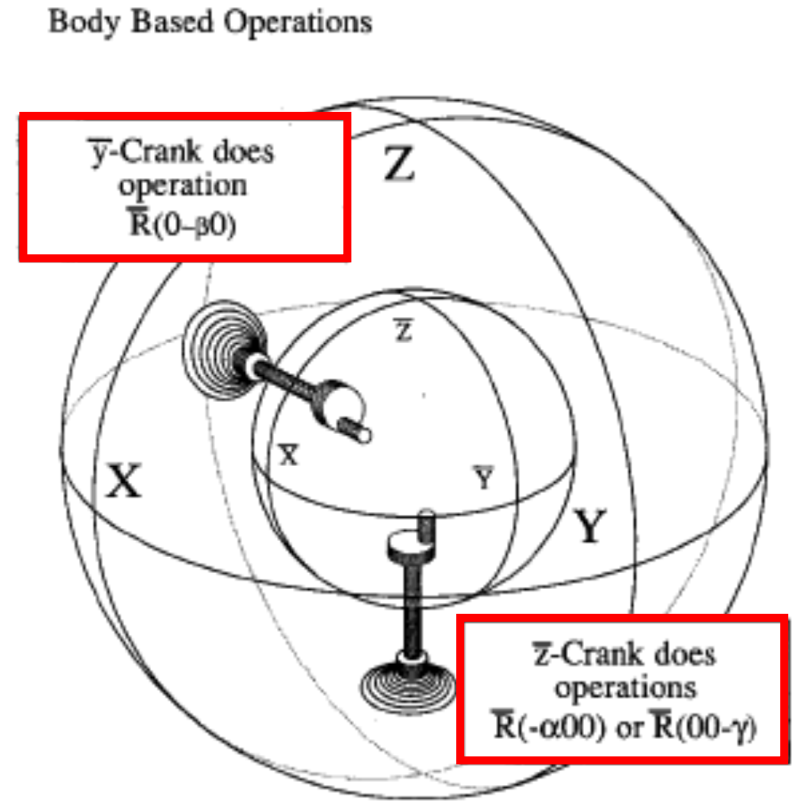


Figure from Ch. 5 of PSDS (Originally in Rev. Mod. Phys. 50, 1, p. 37-83 (1978) Fig. 2)

Review :

Applications of R(3) rotation and U(2) representations

Molecular and nuclear wavefunctions

➡ *Molecular and nuclear eigenlevels* ⬅

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Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high J properties

$$\mathbf{H}_{symmetric\ top} = B\mathbf{J}_{\bar{X}}^2 + B\mathbf{J}_{\bar{Y}}^2 + B\mathbf{J}_{\bar{Z}}^2 + (A-B)\mathbf{J}_{\bar{Z}}^2 = B\mathbf{J}\bullet\mathbf{J} + (A-B)\mathbf{J}_{\bar{Z}}^2$$

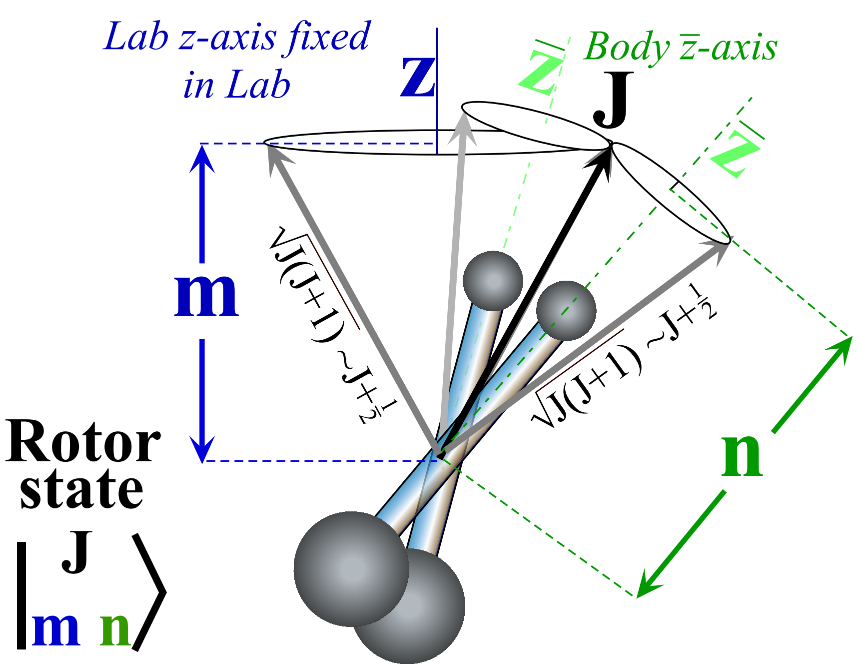
Eigensolution equations:

$$\mathbf{H}_{symmetric\ top}\left|{}^{j}_{m,n}\right\rangle$$

$$= B\mathbf{J}\bullet\mathbf{J} + (A-B)\mathbf{J}_{\bar{Z}}^2\left|{}^{j}_{m,n}\right\rangle$$

$$= \left[BJ(J+1) + (A-B)n^2\right]\left|{}^{j}_{m,n}\right\rangle$$

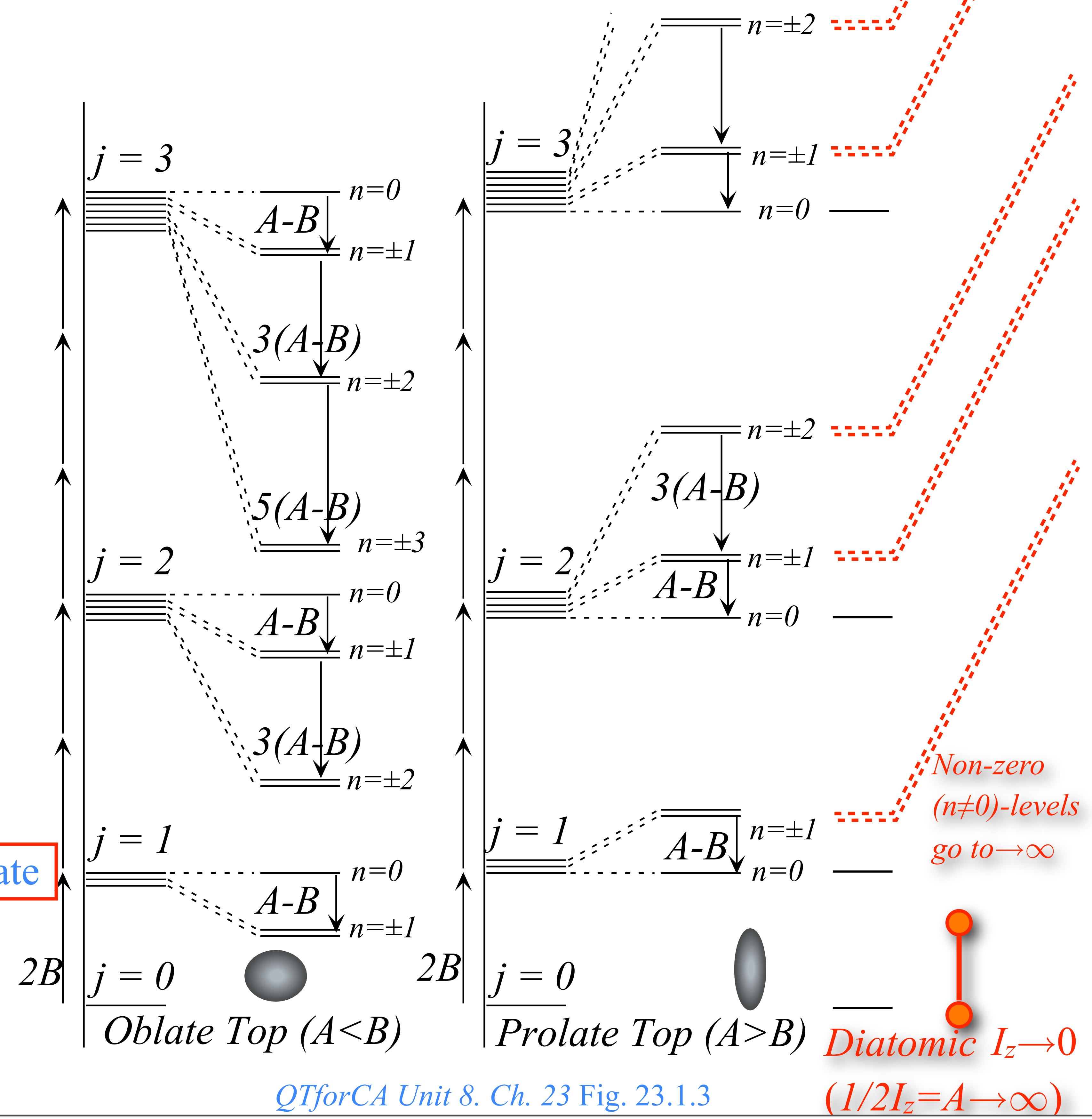
Mock-Mach-Multiplicity
is $(2j+1)^2$ for each j



Even n=0 levels are $2j+1$-fold degenerate

If n is non-zero the degeneracy is $4j+2$.

QTforCA Unit 8. Ch. 23 Fig. 23.2.4



QTforCA Unit 8. Ch. 23 Fig. 23.1.3

Applications of R(3) rotation and U(2) representations

Eigensolution equations:

$$\mathbf{H}_{symmetric\ top}\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$$

$$= B\mathbf{J}\bullet\mathbf{J} + (A-B)\mathbf{J}^2_{\bar{Z}}\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$$

$$= \left[BJ(J+1) + (A-B)n^2\right]\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$$

$$\left|\begin{matrix} j \\ m,n \end{matrix}\right\rangle$$

LAB *BOD*
m=M *n=K*

Conventional notation: n=K

Mock-Mach-Multiplicity is $(2j+1)^2$ for each j

Molecular and nuclear eigenlevels

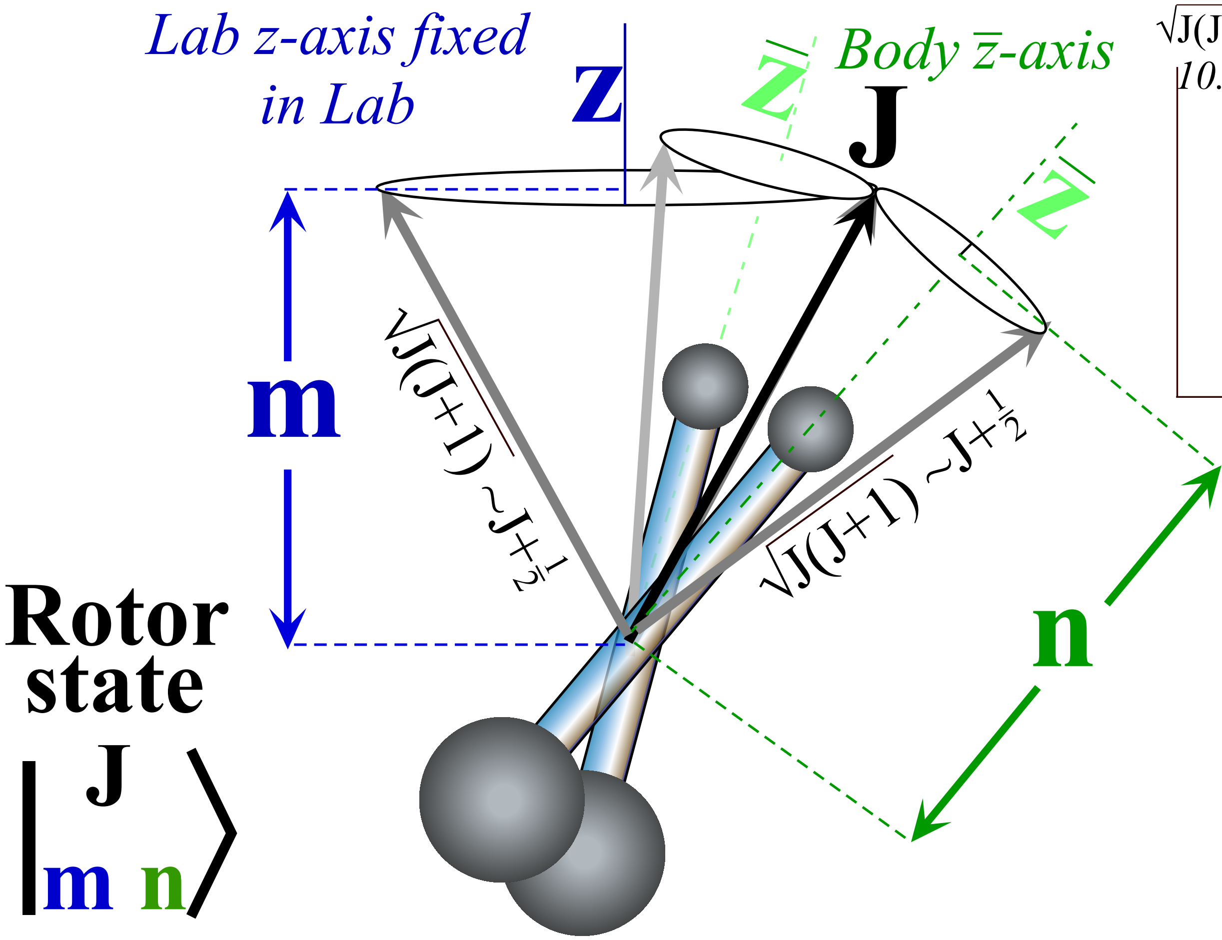
Introducing Racah tensor notation

$$T_0^0 = \mathrm{J}\cdot\mathrm{J} = \langle J\rangle^2 = \left(J_x^2 + J_y^2 + J_y^2\right),$$

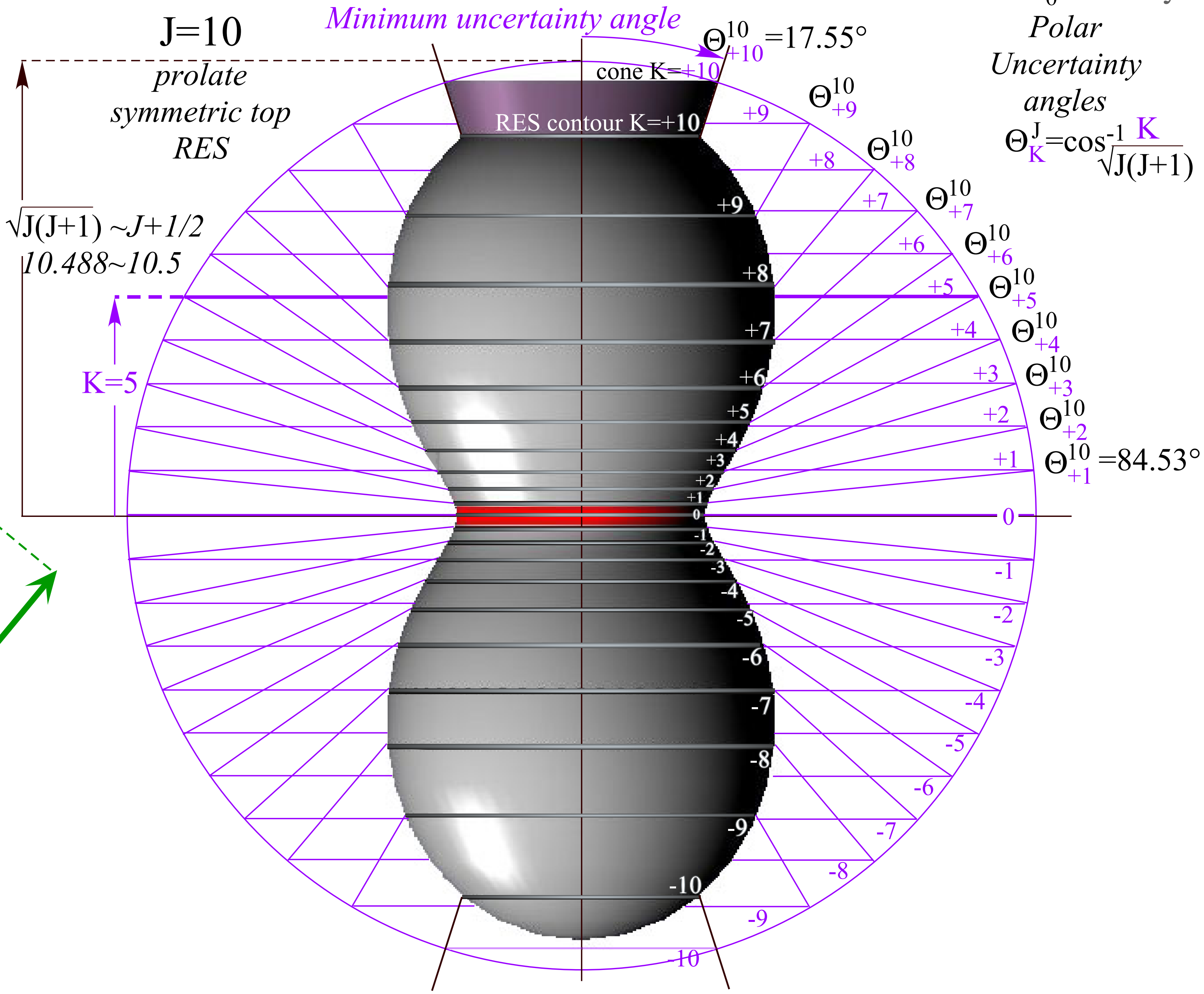
$$T_0^2 = \tfrac{1}{2}\langle J\rangle^2\left(3\cos^2\beta - 1\right) = \tfrac{1}{2}\left(2J_z^2 - J_x^2 - J_y^2\right),$$

$$H = B\ T_0^0 + \frac{2}{3}(A-B)\ T_0^2$$

Rotational Energy Surface (RES)
Plots Hamiltonian $H=T_0^2$ radially.



QTforCA Unit 8. Ch. 23 Fig. 23.2.4



Int.J.Molecular Science 14.(2013) Fig.1 p. 730

Review :

Applications of R(3) rotation and U(2) representations

Molecular and nuclear wavefunctions

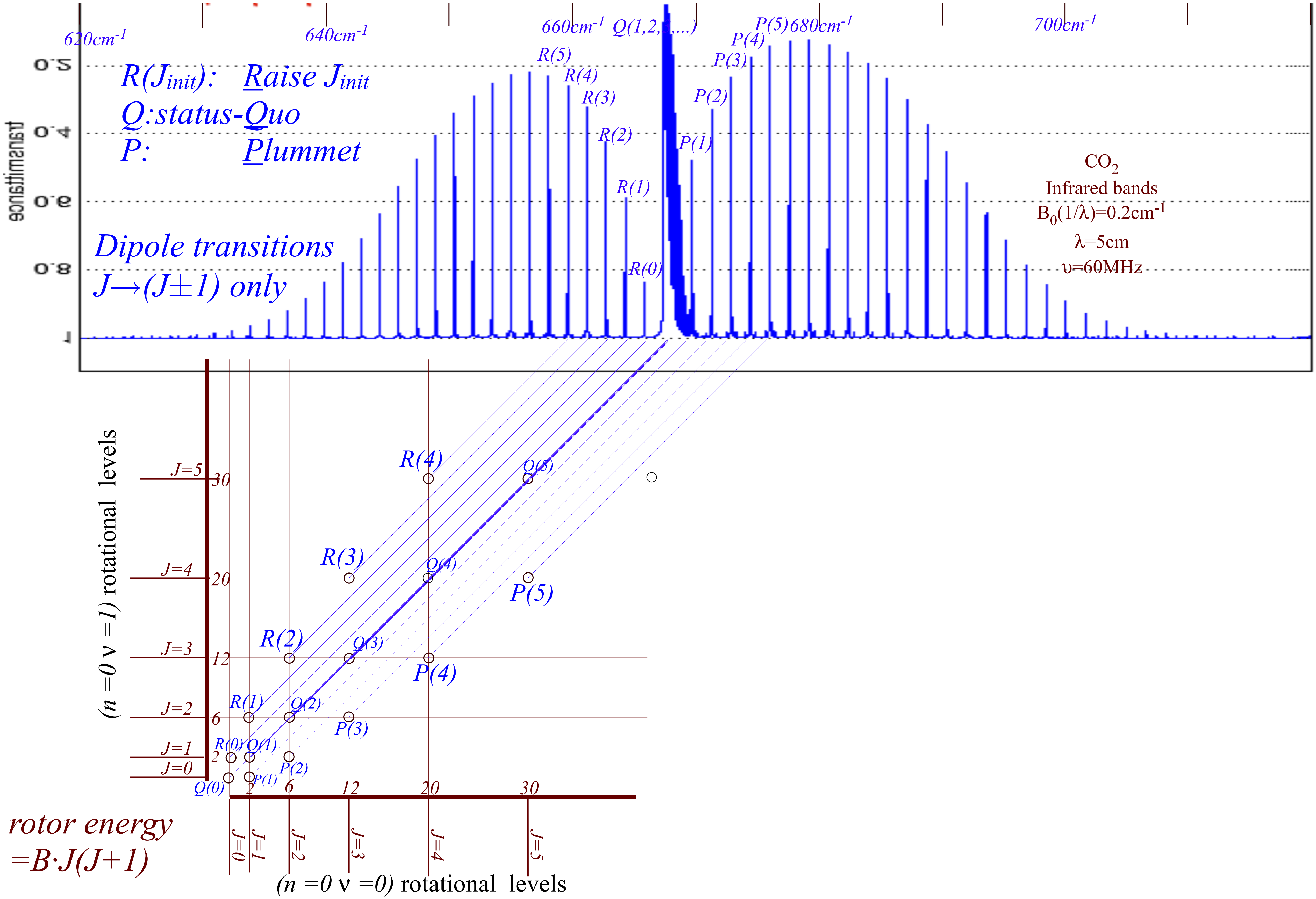
Molecular and nuclear eigenlevels

Example of CO_2 rovibration (υ=0)⇔(υ=1)bands

Generalized Stern-Gerlach and transformation matrices

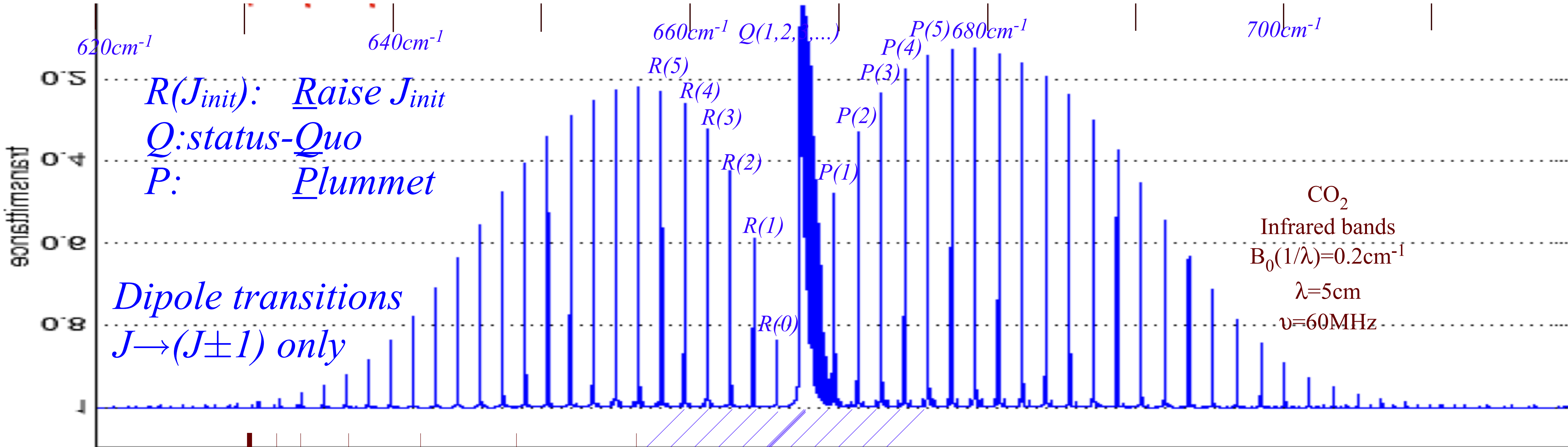
Angular momentum cones and high J properties

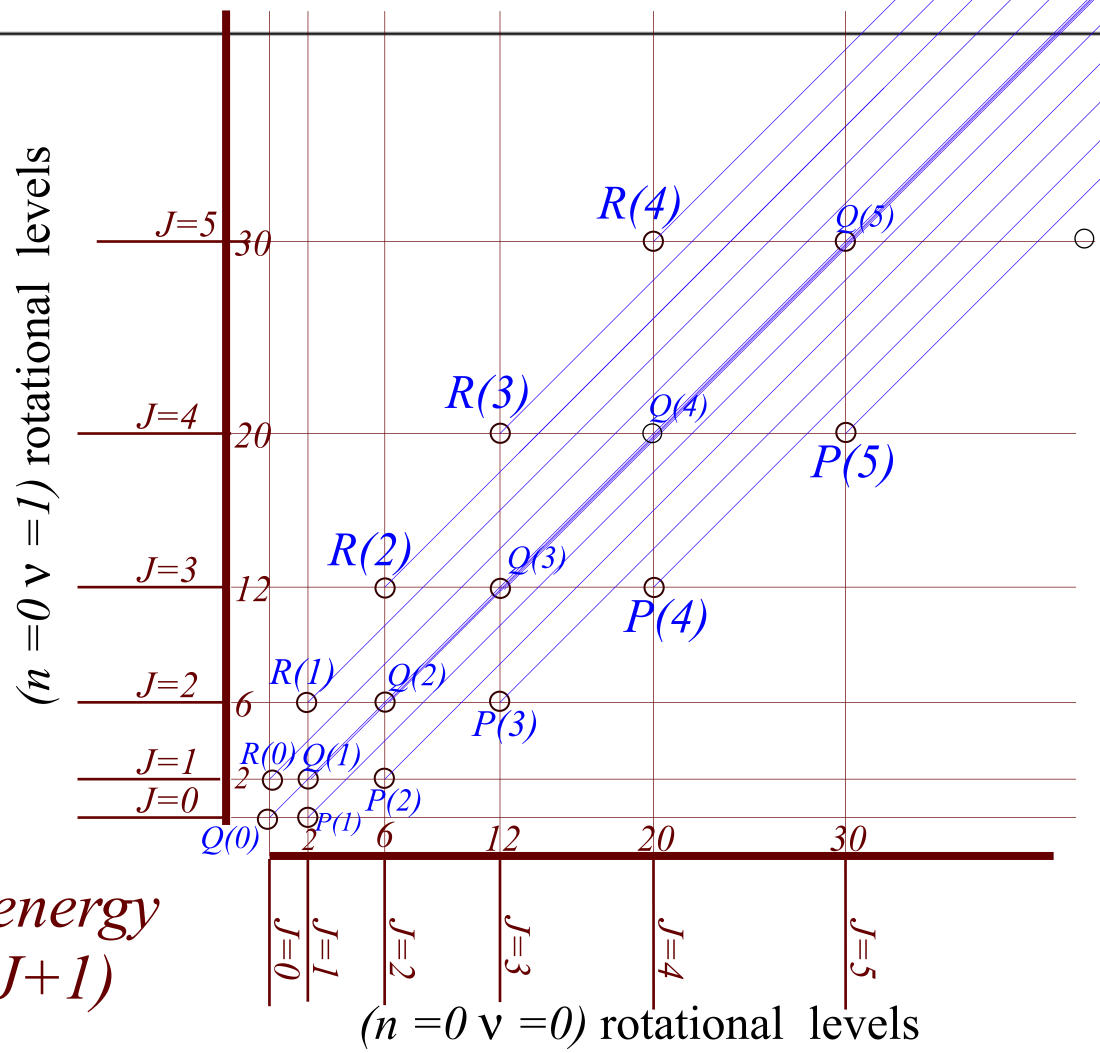
Example of CO_2 rotational (υ=0)⇔(υ=1)bands



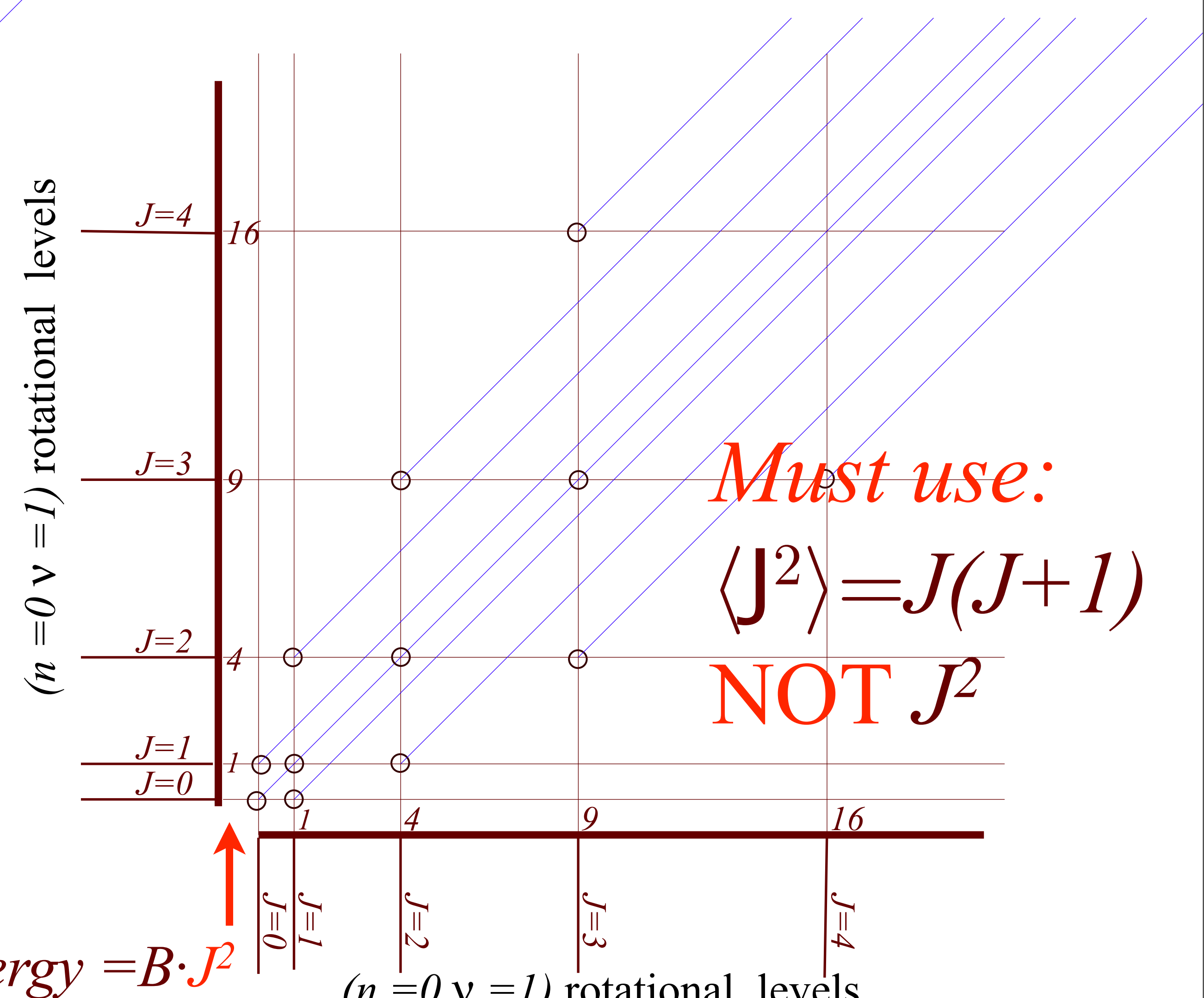
rotor energy
$=B\cdot J(J+1)$

Example of CO_2 rotational $(\upsilon=0)\Leftrightarrow(\upsilon=1)$ bands





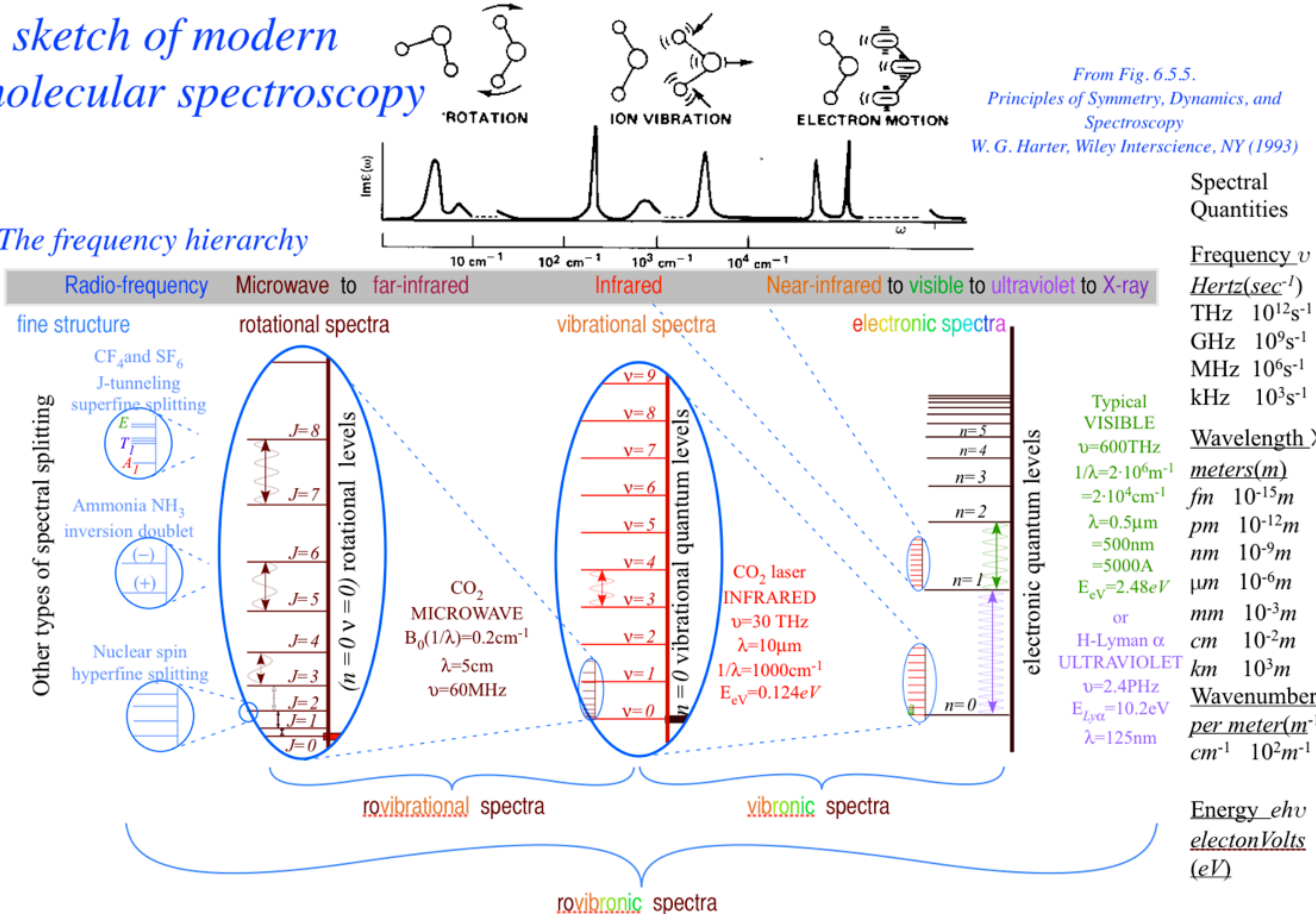
rotor energy $=B\cdot J(J+1)$



Must use:
$\langle \mathbf{J}^2\rangle = J(J+1)$
NOT J^2

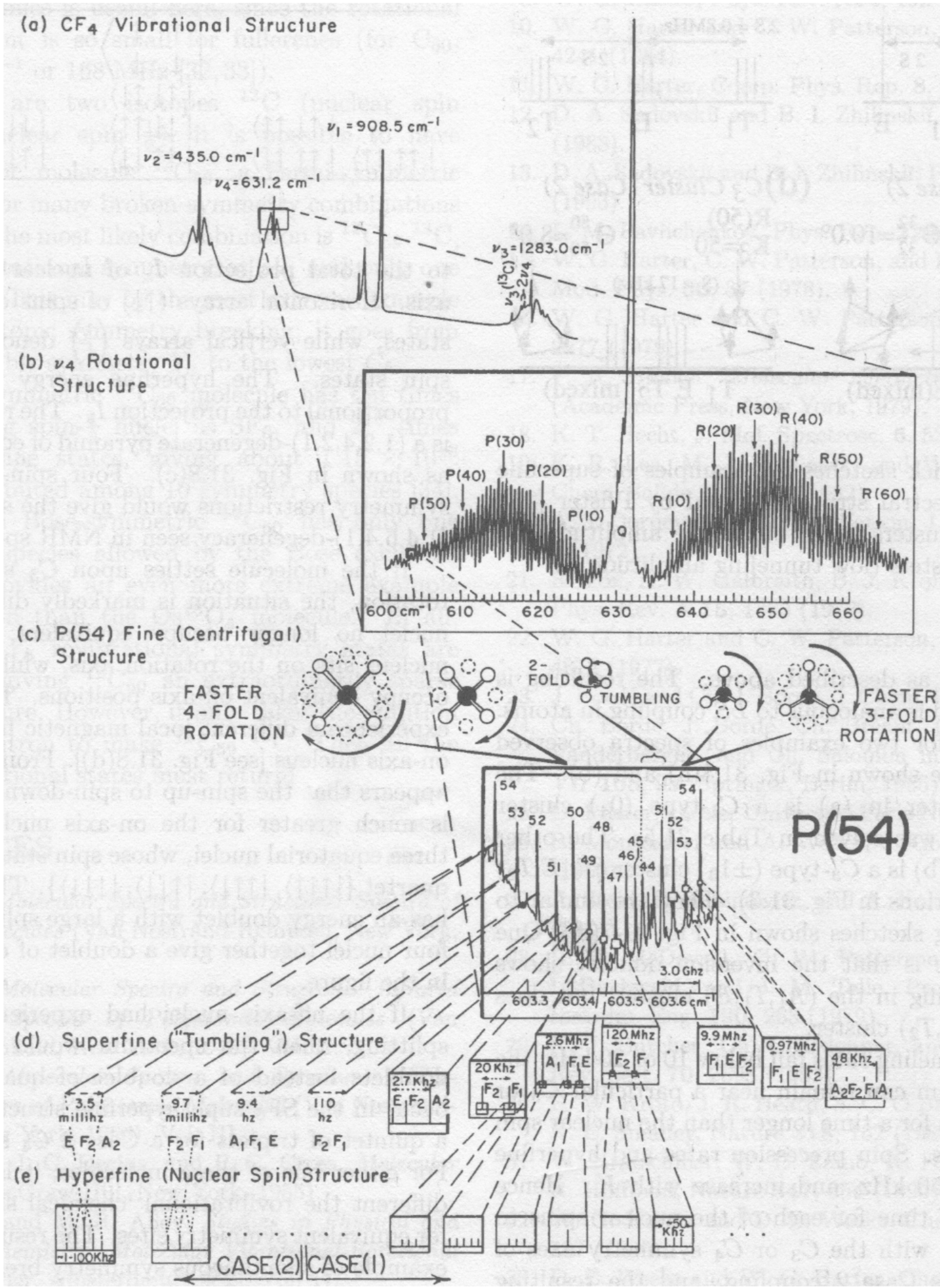
What does NOT work: rotor energy $=B\cdot J^2$

A sketch of modern molecular spectroscopy



Example of frequency hierarchy for 16μm spectra of CF_4 (Freon-14)

W.G.Harter
Ch. 31
Atomic, Molecular, & Optical Physics Handbook
Am. Int. of Physics
Gordon Drake Editor
(1996)



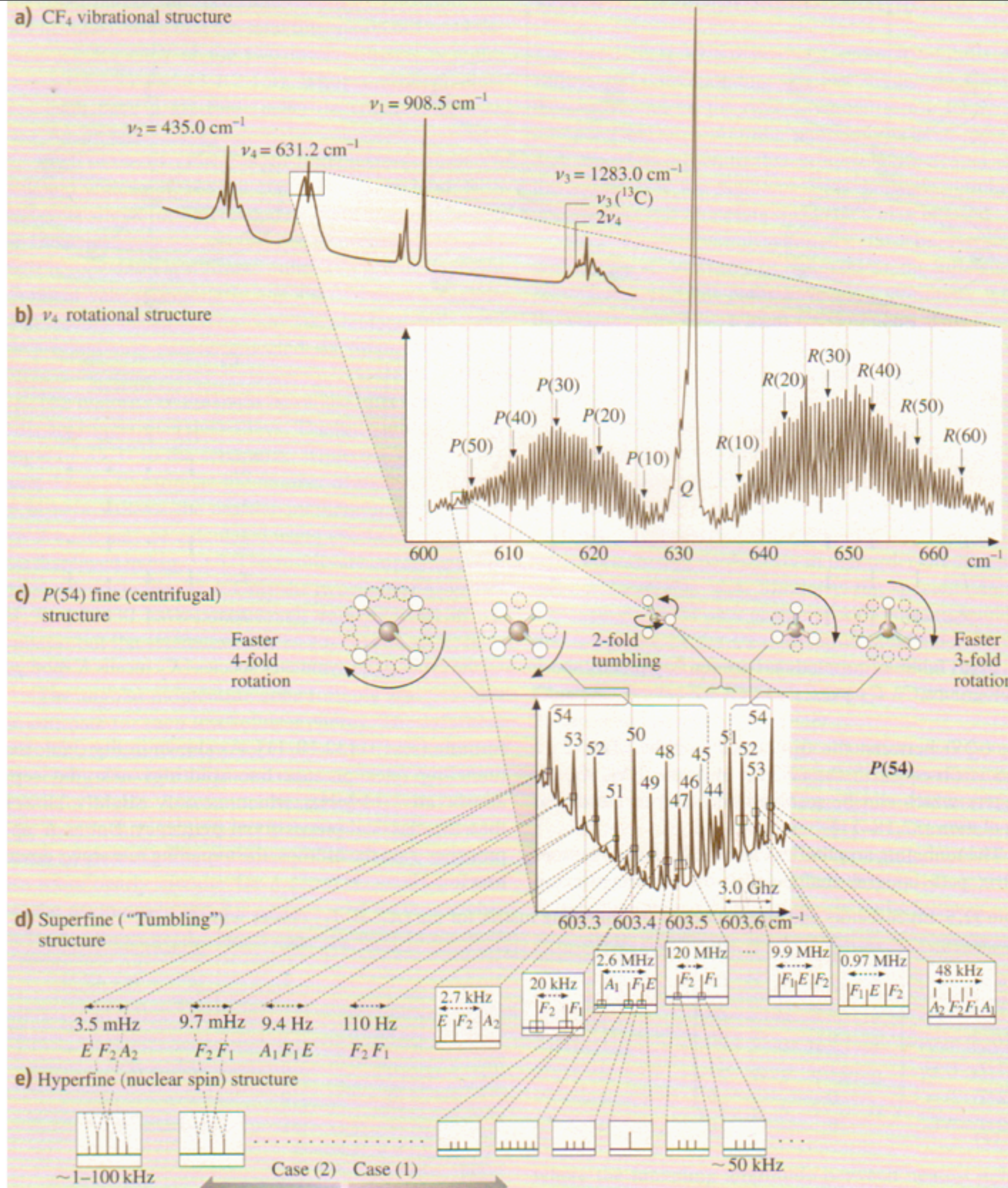
Example of frequency hierarchy for 16μm spectra of CF_4 (Freon-14)

W.G.Harter

Fig. 32.7

Springer Handbook of Atomic, Molecular, & Optical Physics

Gordon Drake Editor (2005)



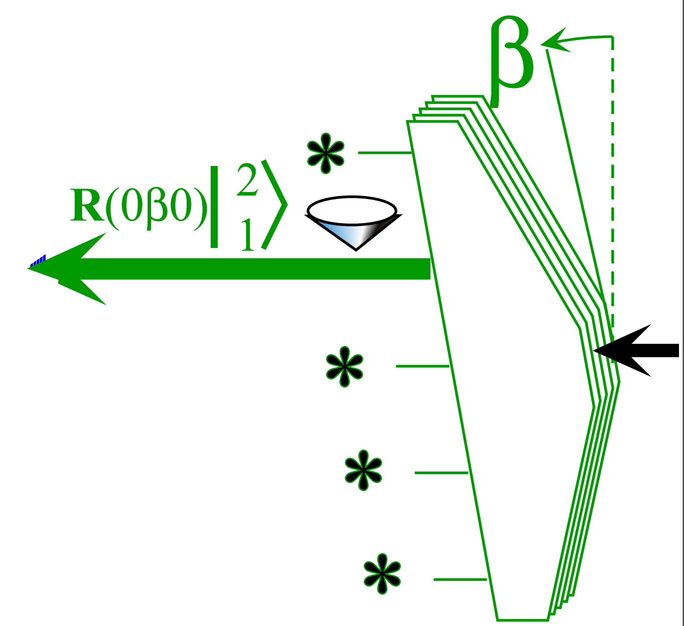
Generalized Stern-Gerlach and transformation matrices

Angular momentum cones and high J properties

Applications of R(3) rotation and U(2) representations

Generalized Stern-Gerlach and transformation matrices

Polarization analysis Suppose a spin-j state $\mathbf{R}(0\beta 0)\left|{}^{j=2}_{m=1}\right\rangle$ exits an analyzer rotated by β



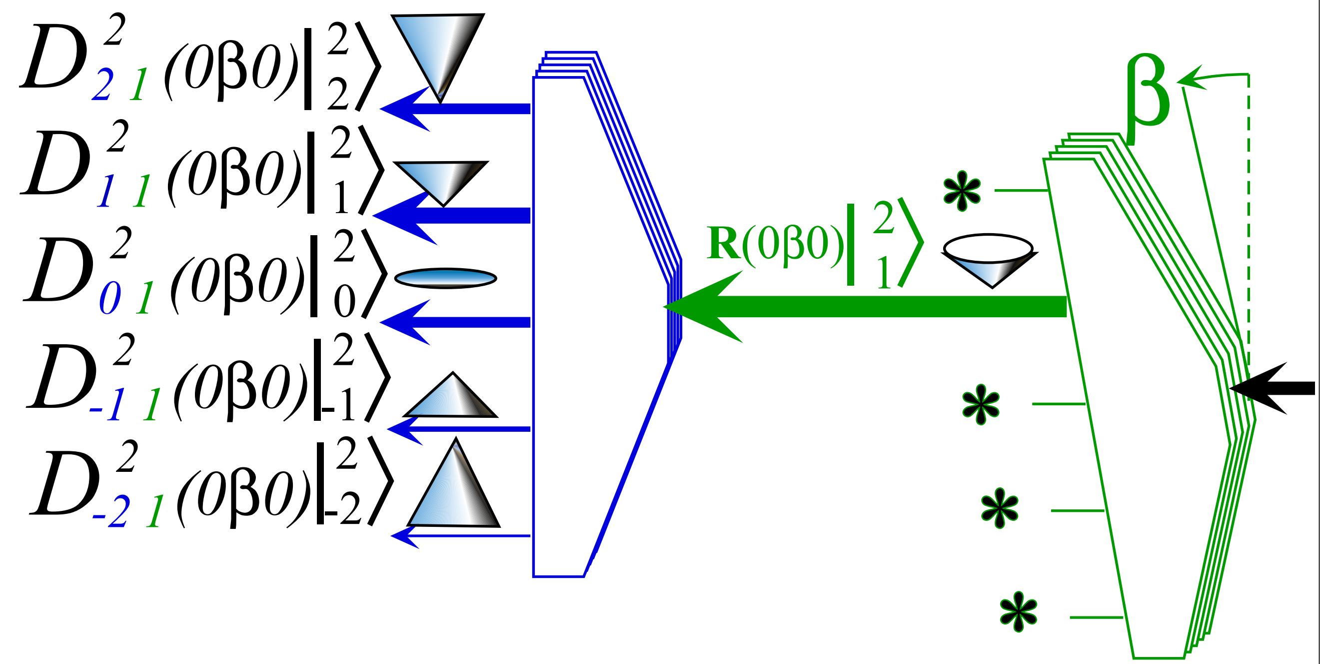
Generalized Stern-Gerlach and transformation matrices

Polarization analysis Suppose a spin-j state $\mathbf{R}(0\beta 0)\,|{}^{j=2}_{m=1}\rangle$ exits an analyzer rotated by β

and then enters a vertical ($\beta=0$) analyzer and forced to choose from unrotated states $|{}^{j=2}_{m'}\rangle$

$$\mathbf{R}(0\beta 0)\left|{}^{j}_{m}\right\rangle = \sum_{m'=-j}^{j} \left|{}^{j}_{m'}\right\rangle \left\langle {}^{j}_{m'}\right| \mathbf{R}(0\beta 0) \left|{}^{j}_{m}\right\rangle$$

$$= \sum_{m'=-j}^{j} \left|{}^{j}_{m'}\right\rangle D^{j}_{m'm}(0\beta 0)$$



QTforCA Unit 8. Ch. 23 Fig. 23.2.1

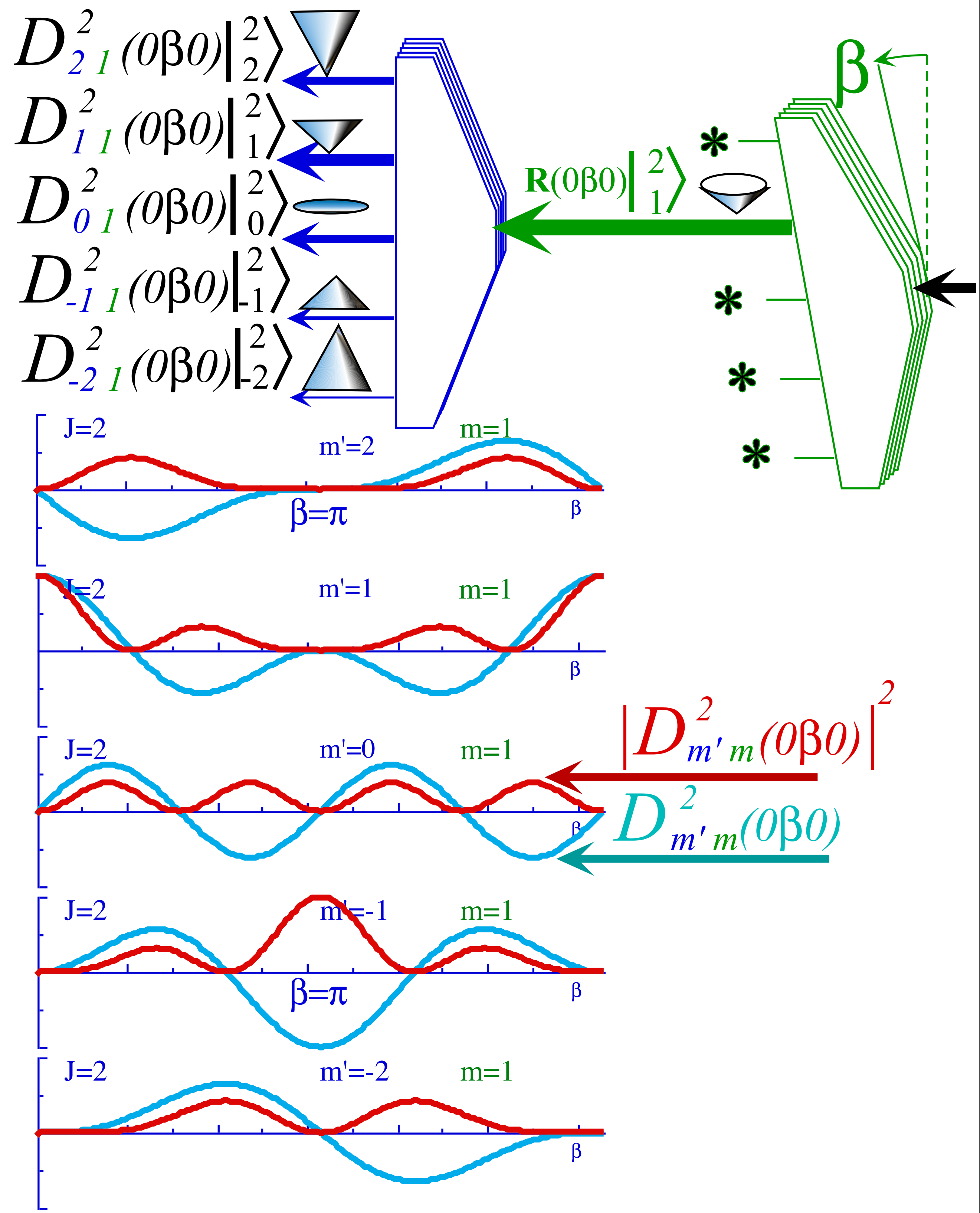
Applications of R(3) rotation and U(2) representations

Generalized Stern-Gerlach and transformation matrices

Polarization analysis Suppose a spin-j state $\mathbf{R}(0\beta 0)\,|^{j=2}_{m=1}\rangle$ exits an analyzer rotated by β and then enters a vertical ($\beta=0$) analyzer and forced to choose from unrotated states $|^{j=2}_{m'}\rangle$

$$\mathbf{R}(0\beta 0)\left|{}^{j}_{m}\right\rangle = \sum_{m'=-j}^{j}\left|{}^{j}_{m'}\right\rangle\left\langle{}^{j}_{m'}\right|\mathbf{R}(0\beta 0)\left|{}^{j}_{m}\right\rangle$$

$$= \sum_{m'=-j}^{j}\left|{}^{j}_{m'}\right\rangle D^{j}_{m'm}(0\beta 0)$$



Overlap of state $\mathbf{R}(\alpha\beta\gamma)\,|^{2}_{1}\rangle$ with unrotated $|^{j=2}_{m'}\rangle$ is the corresponding D-matrix element.

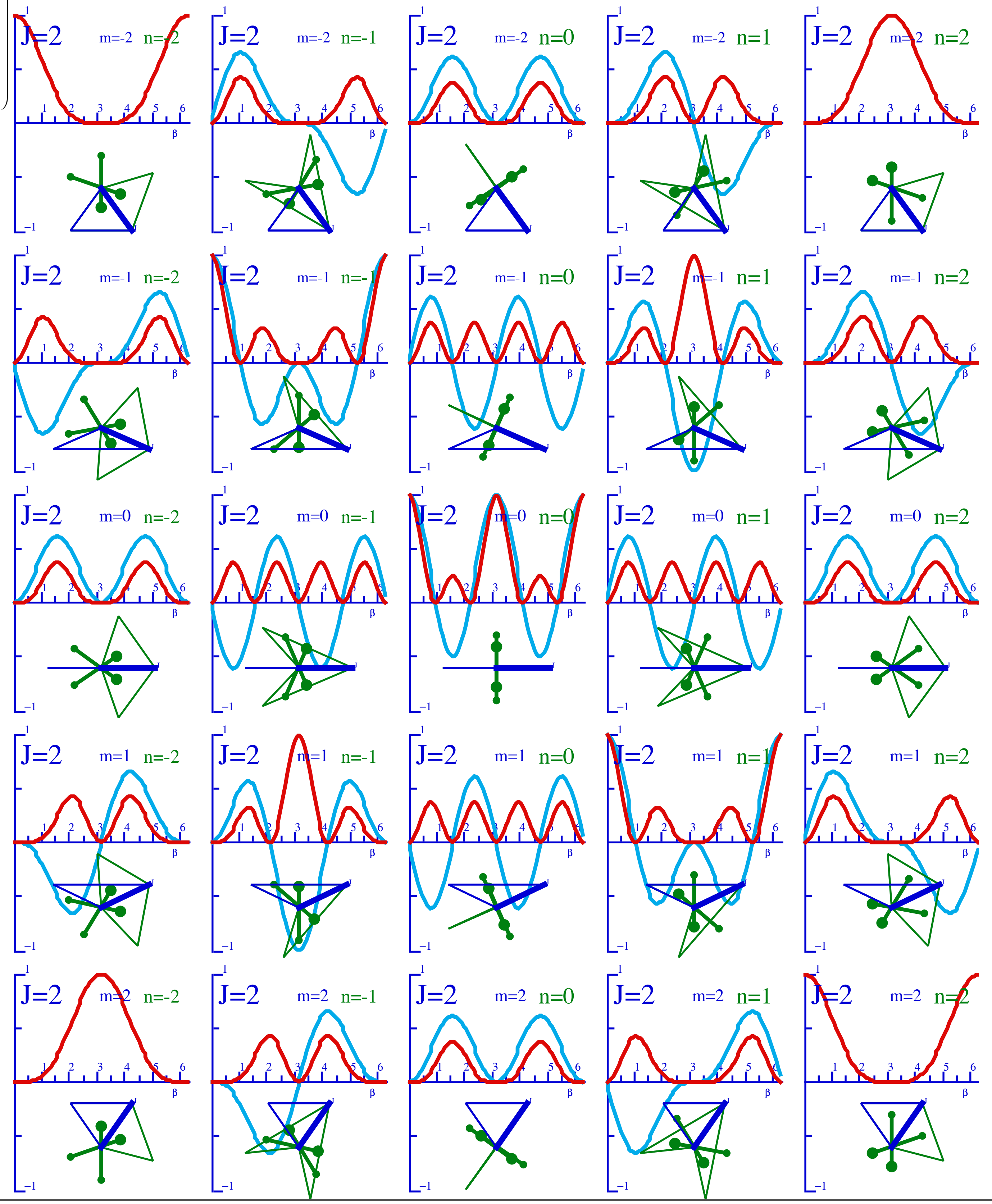
$$\left\langle{}^{j'}_{m'}\right|\mathbf{R}(\alpha\beta\gamma)\left|{}^{2}_{1}\right\rangle = \delta^{j'2} D^{2}_{m'1}(\alpha\beta\gamma) = \left\langle{}^{j'}_{m'}\middle|{}^{2}_{1}\right\rangle_{R}$$

QTforCA Unit 8. Ch. 23 Fig. 23.2.1

$$D^2(\alpha\beta 0)=\left(\begin{array}{cc|c|cc} e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{-i2\alpha}\sin^2\beta & e^{-i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 \\ e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{-i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -\sqrt{\frac{3}{2}}e^{-i\alpha}\sin\beta\cos\beta & e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & -e^{-i\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta \\ \sqrt{\frac{3}{8}}\sin^2\beta & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \frac{3\cos^2\beta-1}{2} & \sqrt{\frac{3}{2}}\sin\beta\cos\beta & \sqrt{\frac{3}{8}}\sin^2\beta \\ e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i\alpha}\left(\frac{1-\cos\beta}{2}\right)(2\cos\beta+1) & \sqrt{\frac{3}{2}}e^{i\alpha}\sin\beta\cos\beta & e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)(2\cos\beta-1) & -e^{i\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta \\ e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)^2 & e^{i2\alpha}\left(\frac{1-\cos\beta}{2}\right)\sin\beta & \sqrt{\frac{3}{8}}e^{i2\alpha}\sin^2\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)\sin\beta & e^{i2\alpha}\left(\frac{1+\cos\beta}{2}\right)^2 \end{array}\right)$$

$$\mathbf{R}(0\beta 0)\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle = \sum_{m'=-j}^{j}\left|\begin{smallmatrix} j \\ m' \end{smallmatrix}\right\rangle\left\langle\begin{smallmatrix} j \\ m' \end{smallmatrix}\right|\mathbf{R}(0\beta 0)\left|\begin{smallmatrix} j \\ m \end{smallmatrix}\right\rangle$$

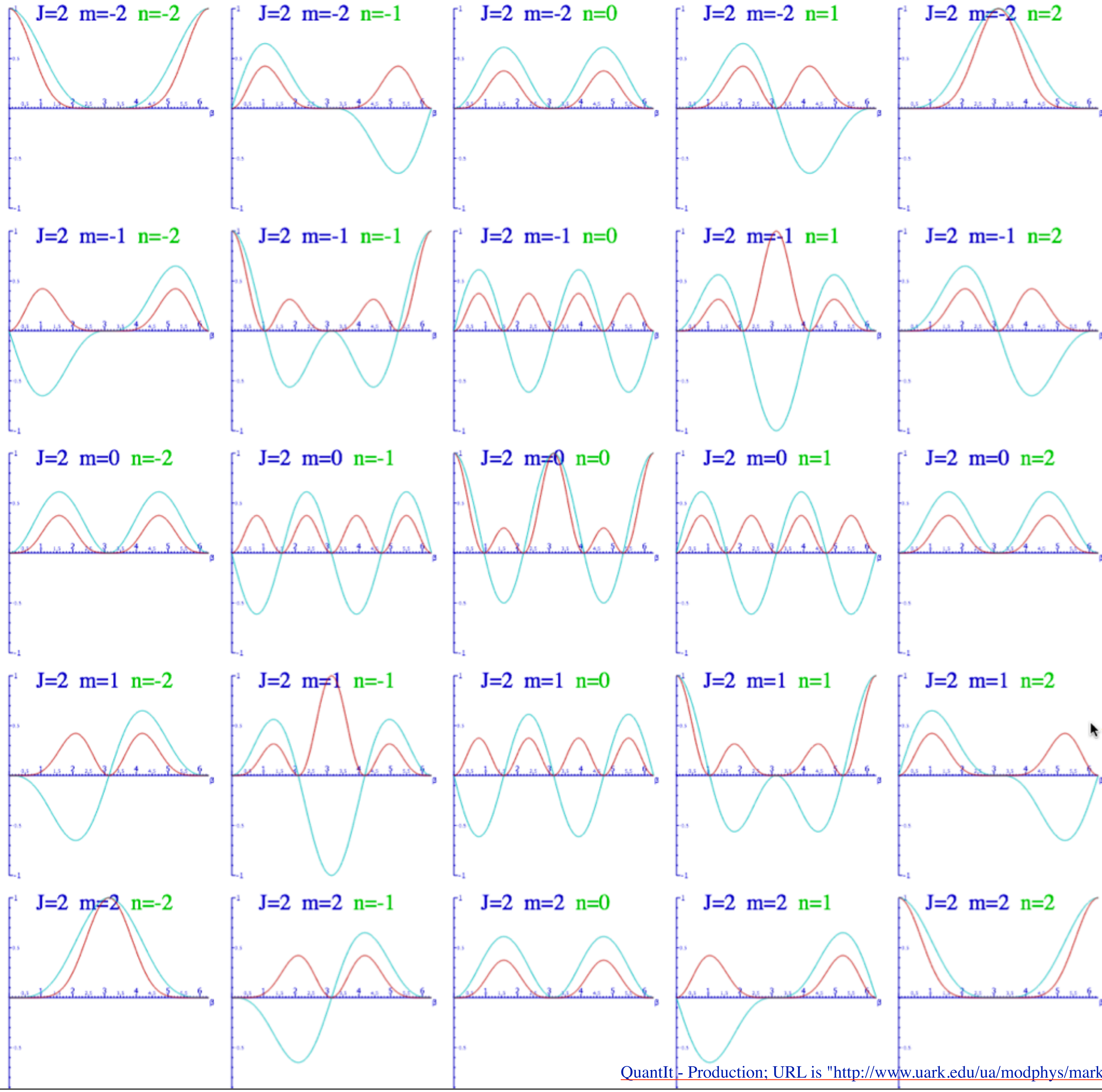
$$= \sum_{m'=-j}^{j}\left|\begin{smallmatrix} j \\ m' \end{smallmatrix}\right\rangle D^j_{m'm}(0\beta 0)$$



Overlap of state $\mathbf{R}(\alpha\beta\gamma)\,|^2{}_1\rangle$ with unrotated $|^{j=2}{}_{m'}\rangle$ is the corresponding D-matrix element.

$$\left\langle\begin{smallmatrix} j' \\ m' \end{smallmatrix}\right|\mathbf{R}(\alpha\beta\gamma)\left|\begin{smallmatrix} 2 \\ 1 \end{smallmatrix}\right\rangle = \delta^{j'2}D^2_{m'1}(\alpha\beta\gamma) = \left\langle\begin{smallmatrix} j' \\ m' \end{smallmatrix}\middle|\begin{smallmatrix} 2 \\ 1 \end{smallmatrix}\right\rangle_R$$

QTforCA Unit 8. Ch. 23 Fig. 23.2.5

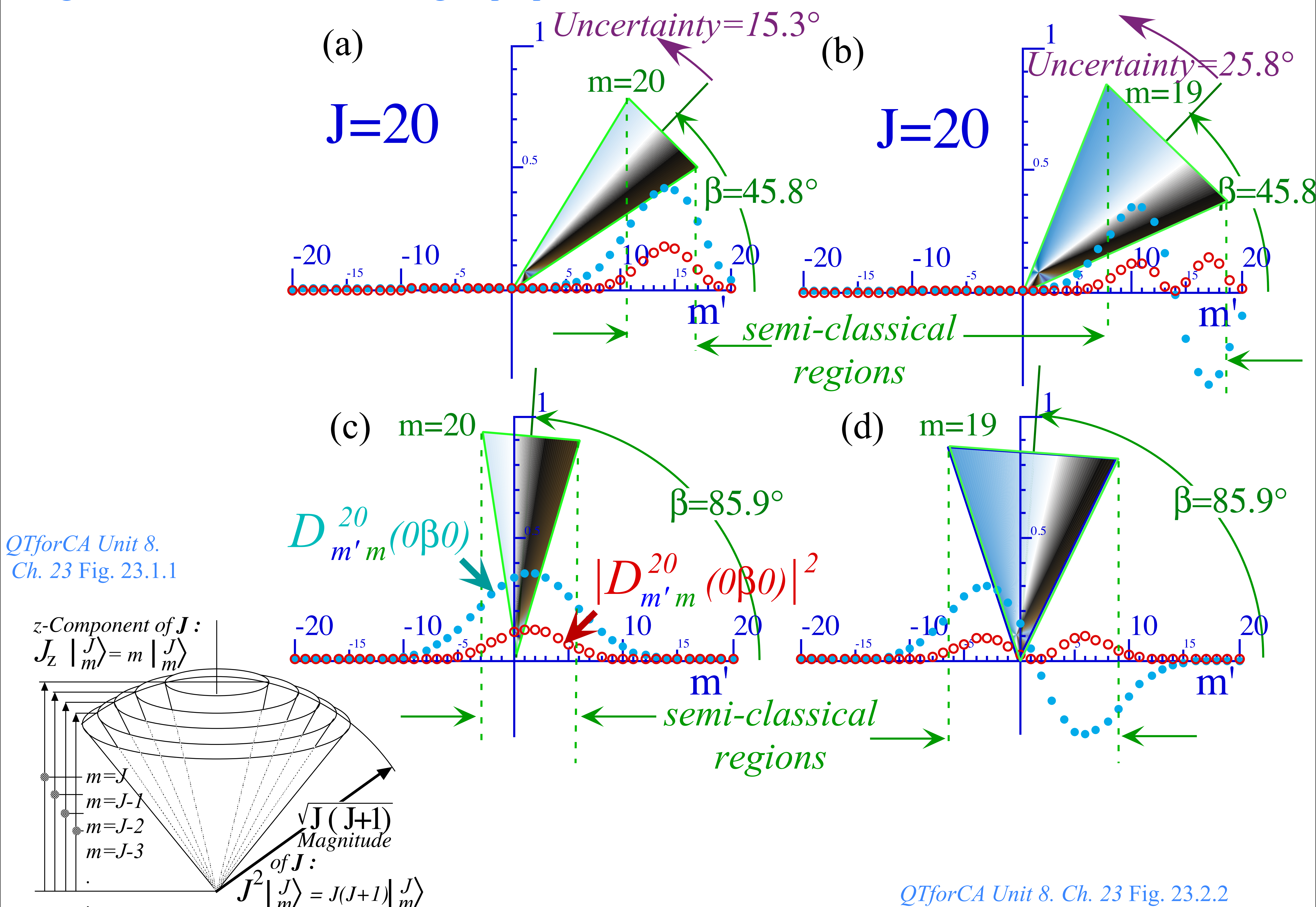


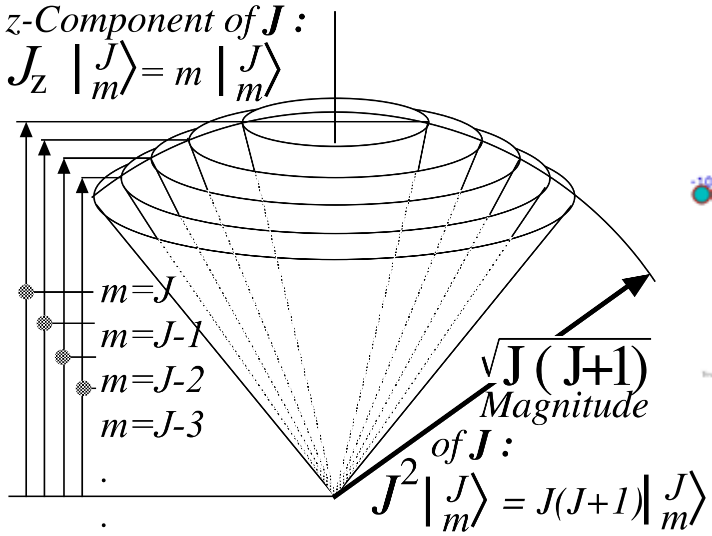
QuantIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"

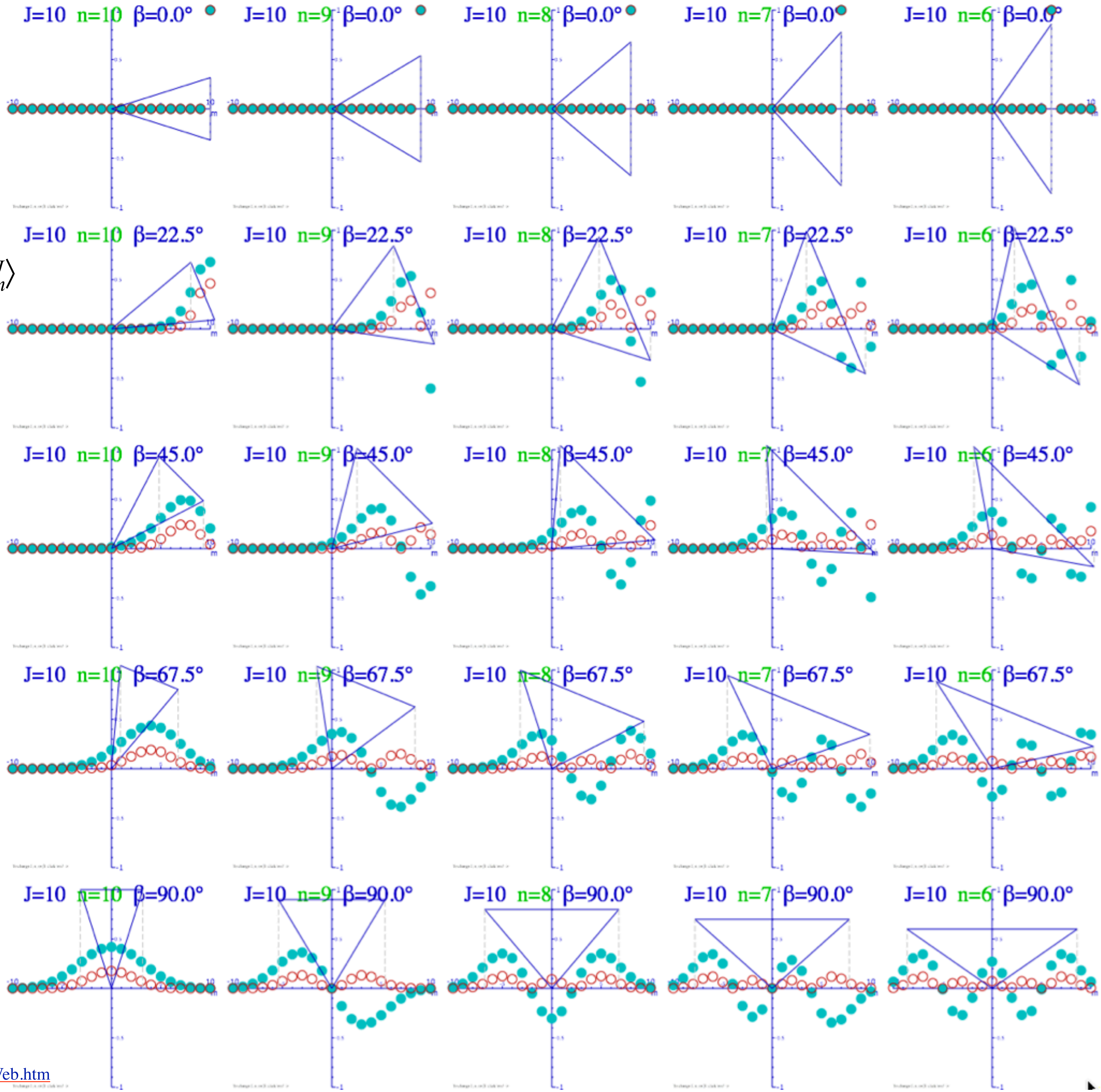
Generalized Stern-Gerlach and transformation matrices

→ *Angular momentum cones and high J properties* ←

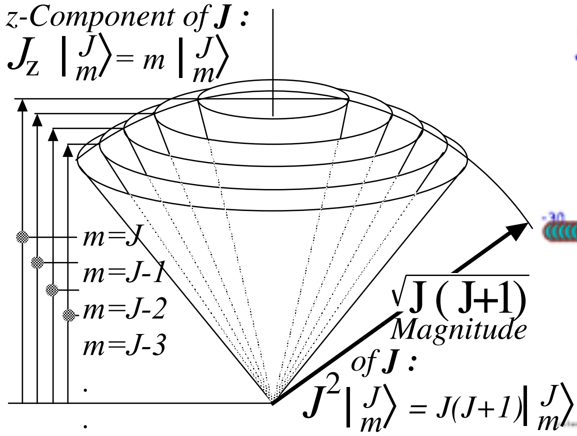
Angular momentum cones and high J properties

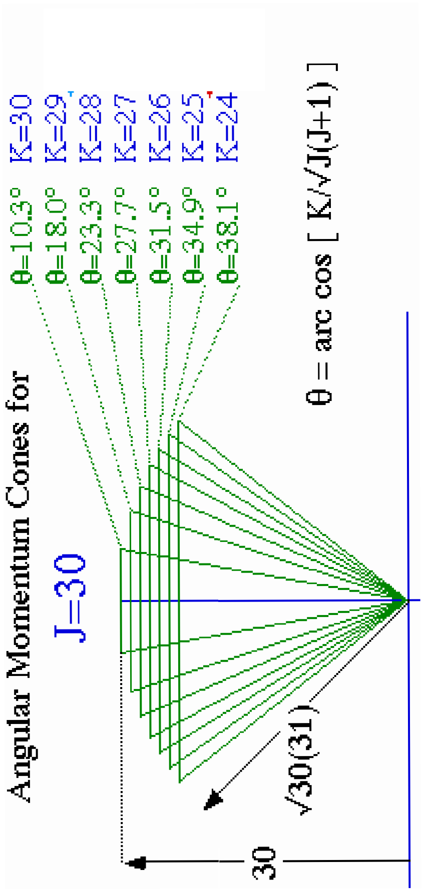


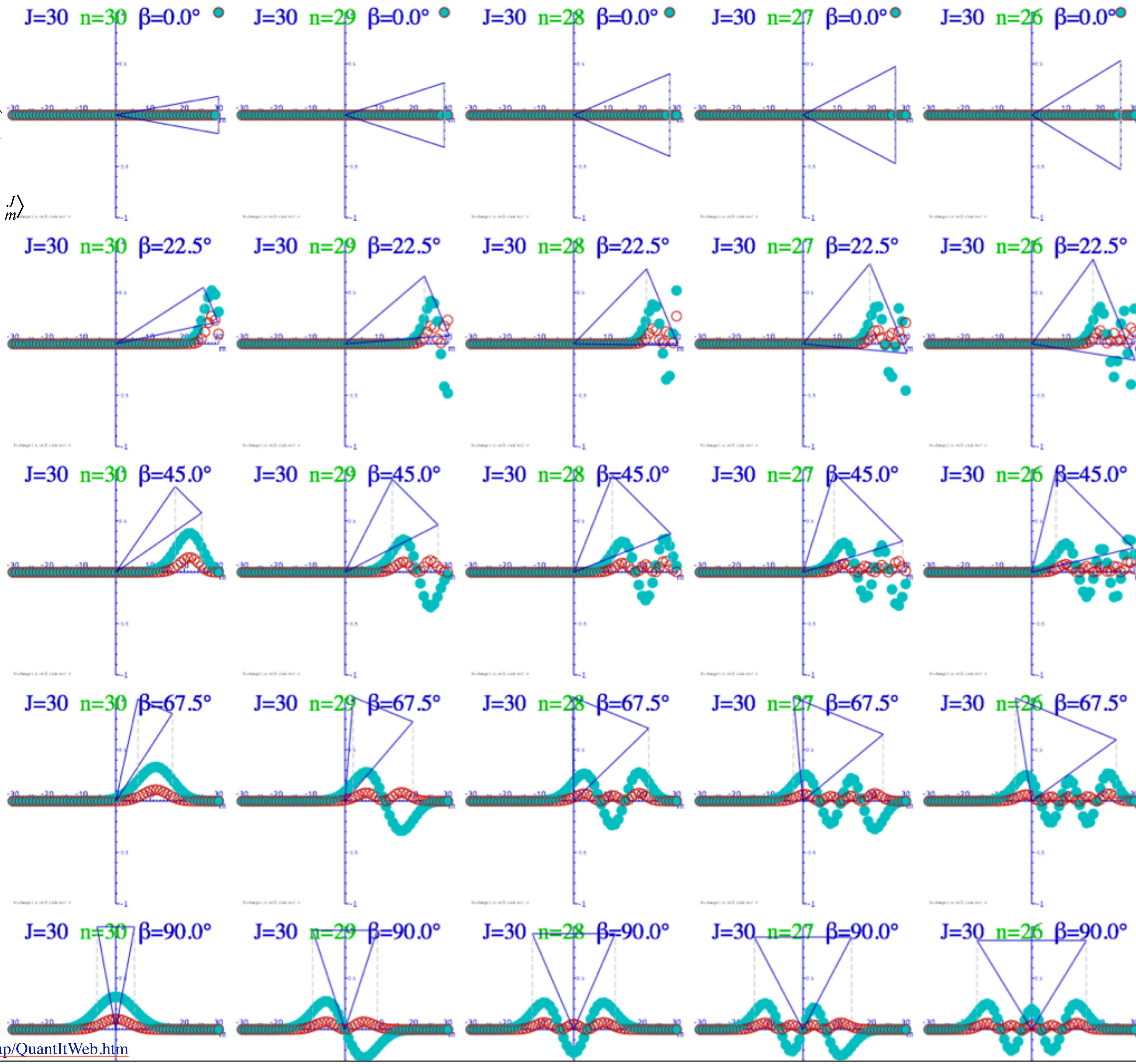




http://www.uark.edu/ua/modphys/markup/QuantItWeb.htm

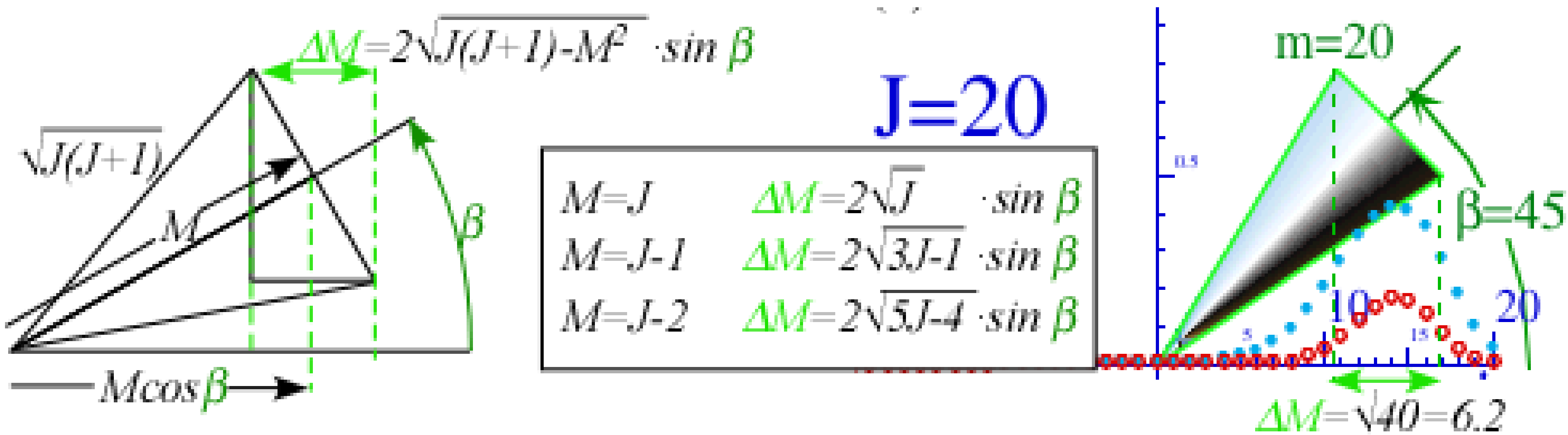






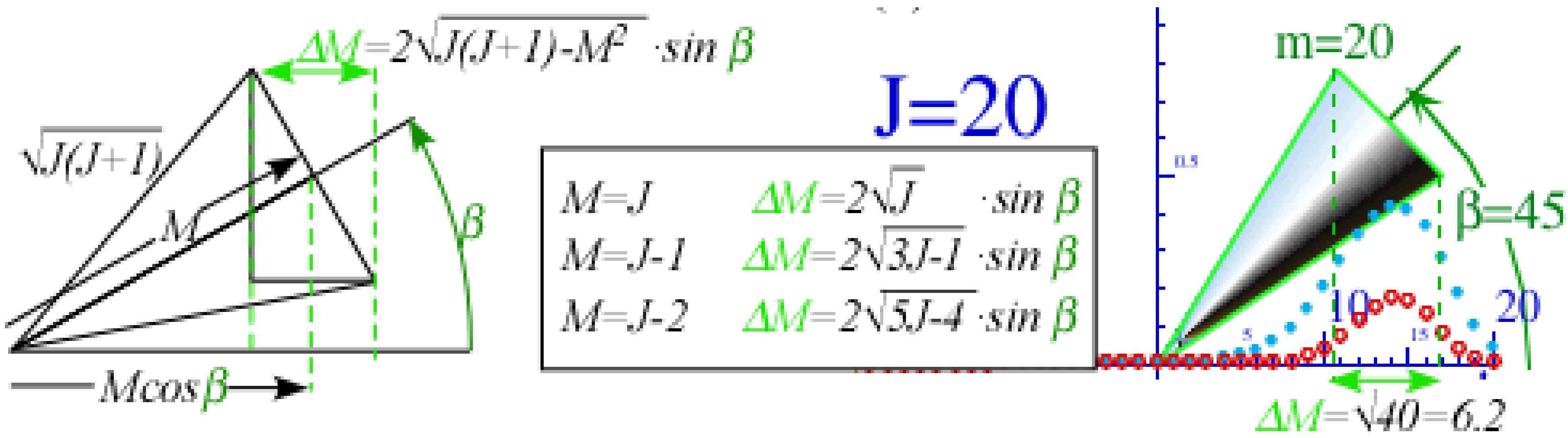
http://www.uark.edu/ua/modphys/markup/QuantItWeb.htm

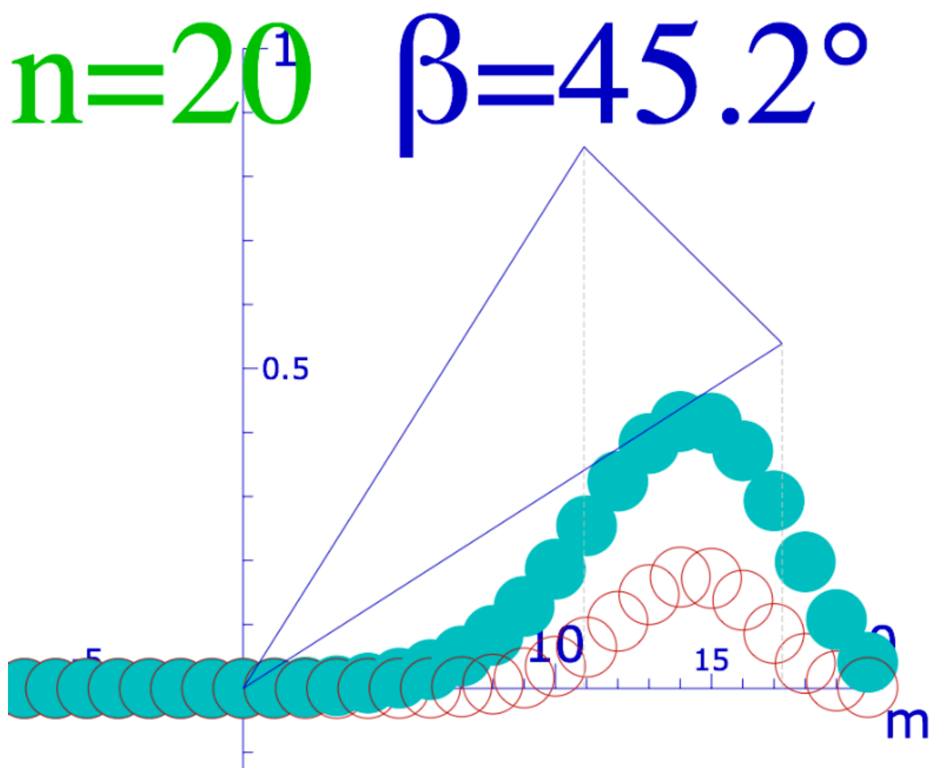
Using literal interpretation of $\left|\begin{smallmatrix}J\\M\end{smallmatrix}\right\rangle$ to derive approximate number ΔM of “most-busy” counters and determine most probable M-value.



Testing formula with $J=20$ for $\beta=45°$...

Using literal interpretation of $\left| {J \atop M} \right\rangle$ to derive approximate number ΔM of "most-busy" counters and determine most probable M-value.

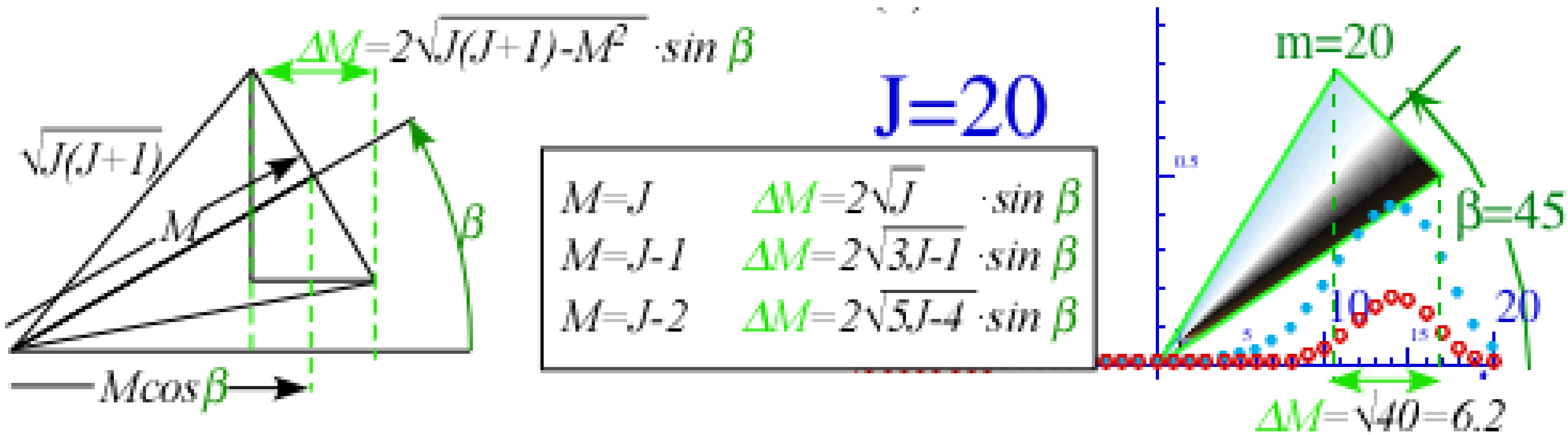


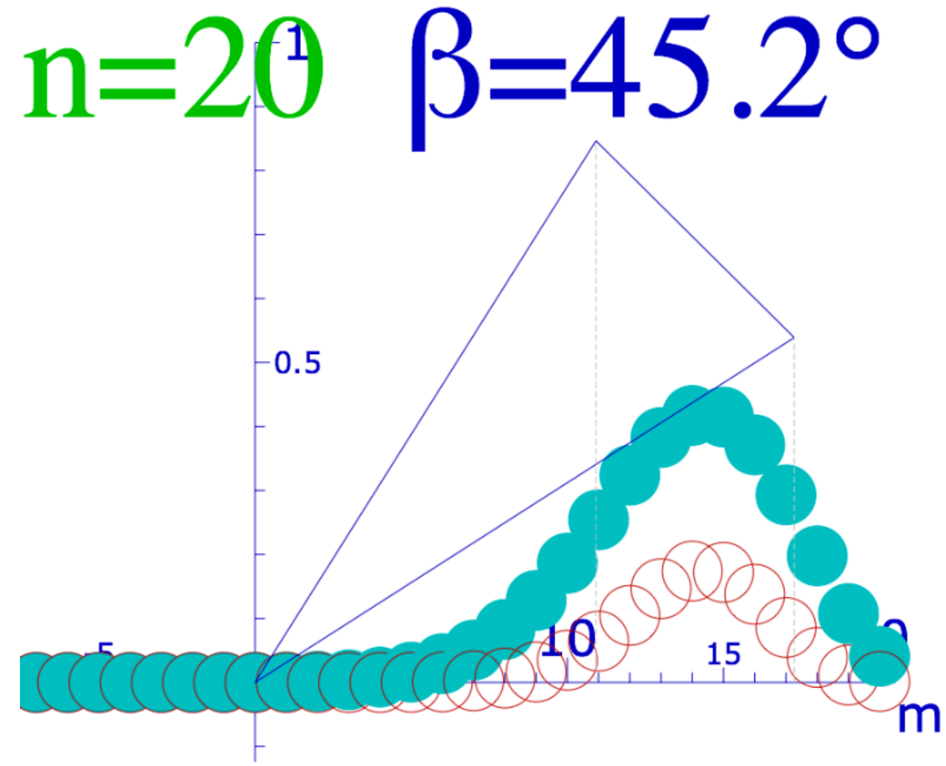


Testing formula with $J=20$ for $\beta=45°$...

http://www.uark.edu/ua/modphys/markup/QuantItWeb.htm

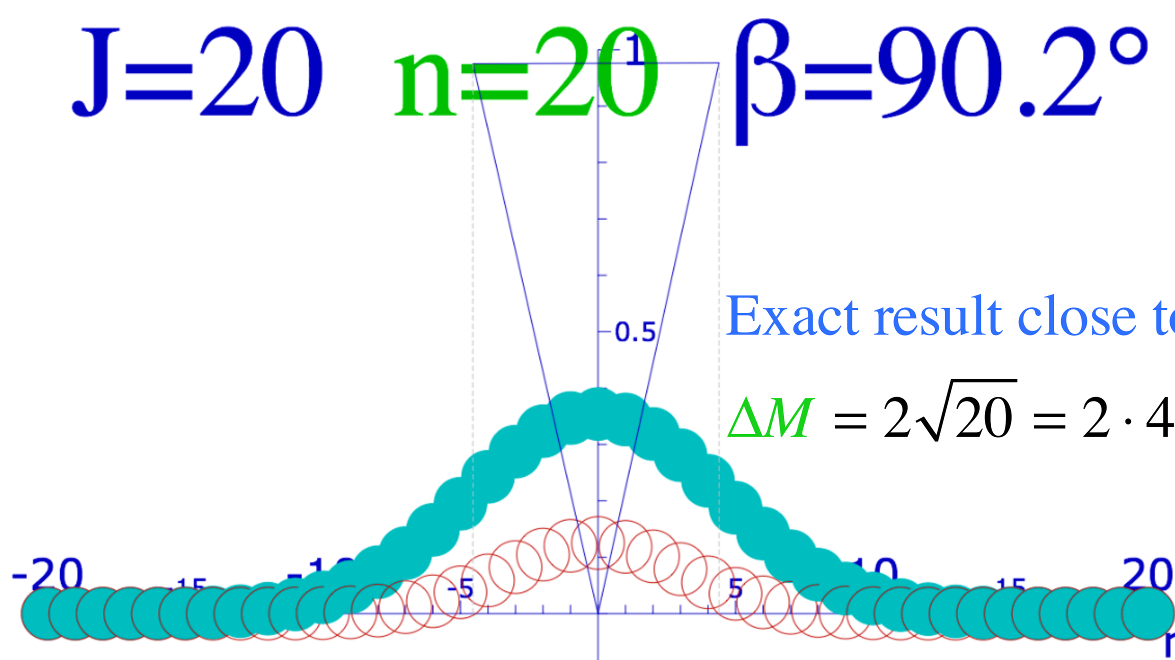
Using literal interpretation of $\left|{J \atop M}\right\rangle$ to derive approximate number ΔM of "most-busy" counters and determine most probable M-value.





Testing formula with $J=20$ for $\beta=45°$...

...and for $\beta=90°$



Exact result close to:

$$\Delta M = 2\sqrt{20} = 2 \cdot 4.47 = 8.94$$

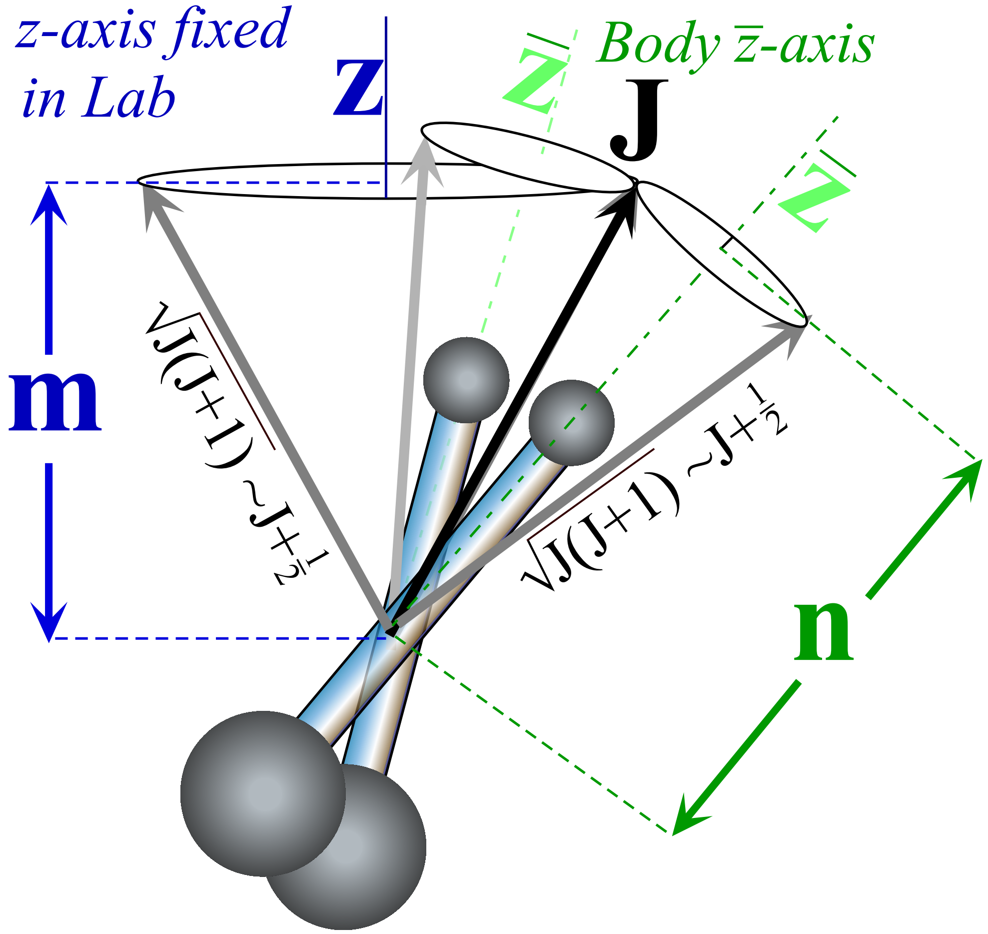
http://www.uark.edu/ua/modphys/markup/QuantItWeb.htm

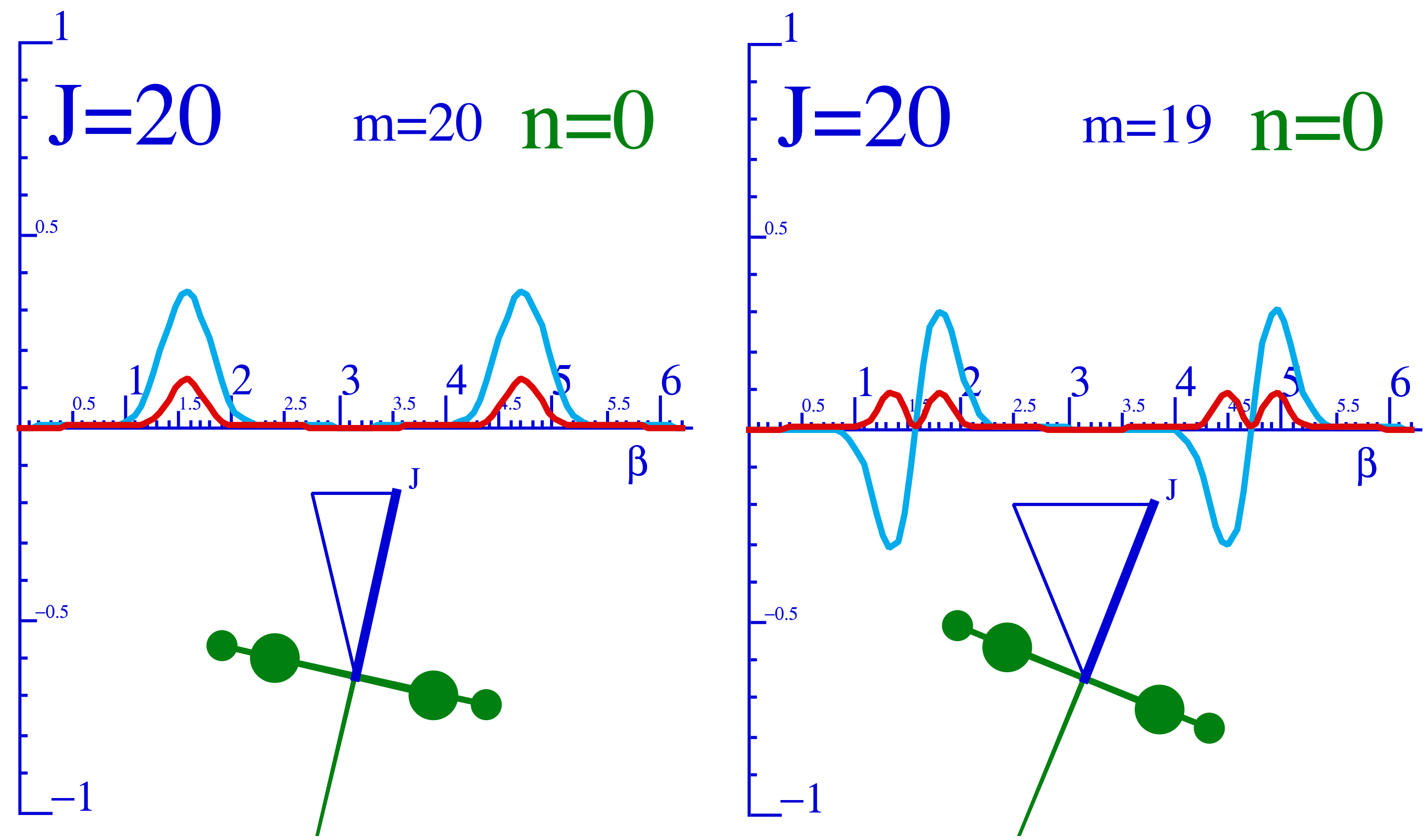
Generalized Stern-Gerlach and transformation matrices

➡ *Angular momentum cones and high J properties*

Using literal interpretation of $\left|\begin{matrix} J \\ m\ n \end{matrix}\right\rangle$ to describe approximate rotor wave-functions

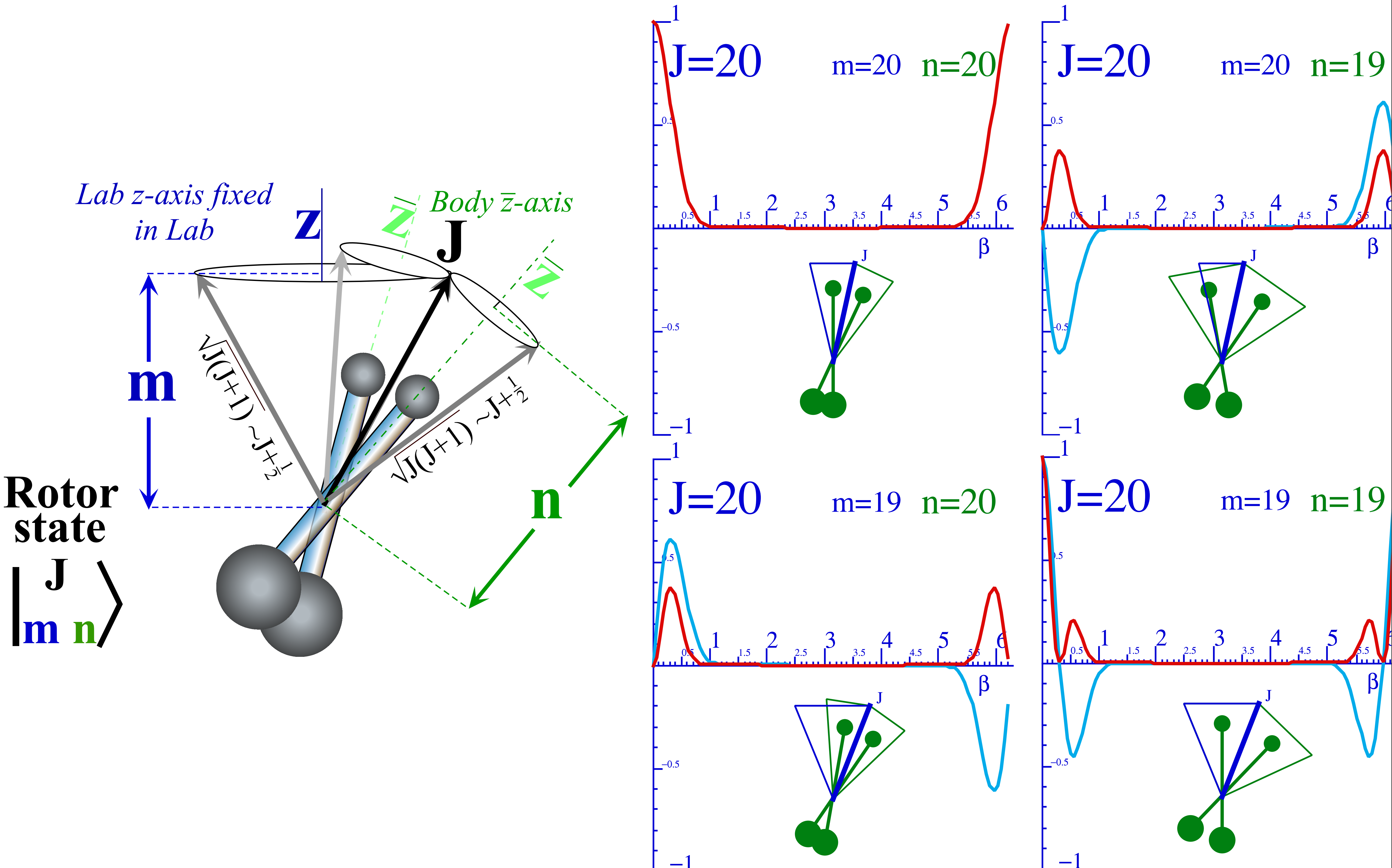
Rotor state $\left|\begin{matrix} J \\ m\ n \end{matrix}\right\rangle$



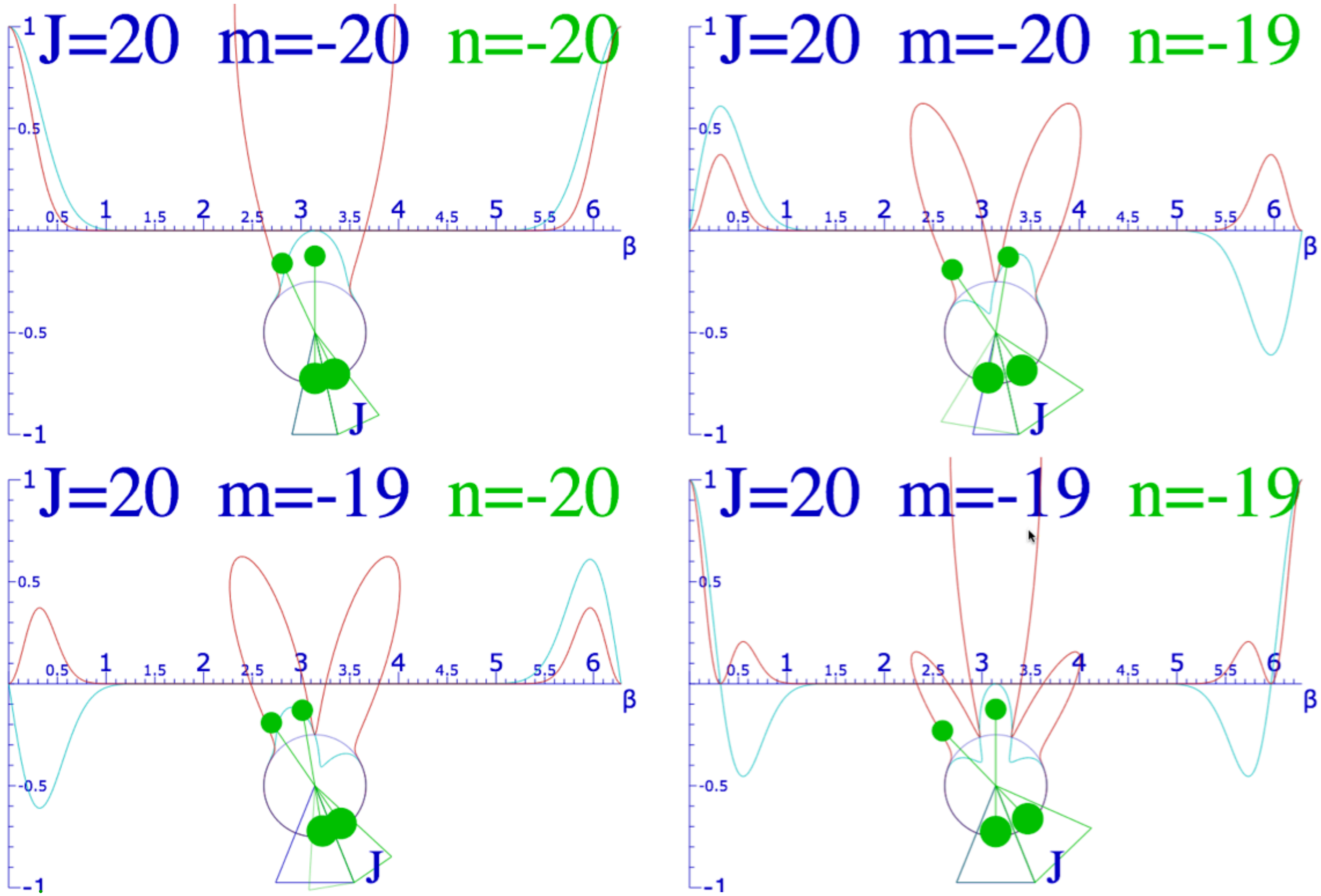


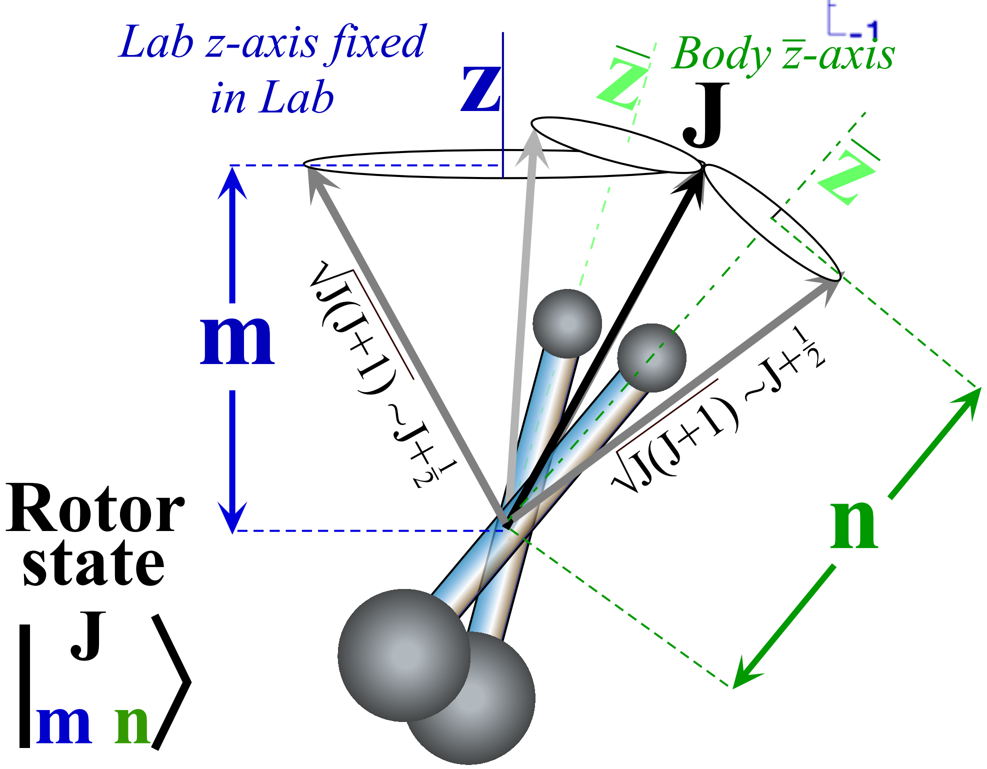
QTforCA Unit 8. Ch. 23 Fig. 23.2.4

QTforCA Unit 8. Ch. 23 Fig. 23.2.7



Lab z-axis fixed in Lab
z
Body z̄-axis
z̄
J
m
n
√J(J+1) ~J+½
Rotor state
|J m n⟩
J=20 m=20 n=20
J=20 m=20 n=19
J=20 m=19 n=20
J=20 m=19 n=19
β





http://www.uark.edu/ua/modphys/markup/QuantItWeb.htm

Asymmetric Top spectra J=1-2

j,m,n formulas for momentum operator matrix elements:

LAB matrix elements use the usual atomic formula:

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_1 \middle| {J \atop m,n} \right\rangle = D^J_{m',m}(\mathbf{J}_1)\delta_{n'n} = \tfrac{1}{2}\left[\delta_{m'm+1}\sqrt{(j-m)(j+m+1)} + \delta_{m'm-1}\sqrt{(j+m)(j-m+1)}\right]\delta_{n'n}$$

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_2 \middle| {J \atop m,n} \right\rangle = D^J_{m',m}(\mathbf{J}_2)\delta_{n'n} = \tfrac{-i}{2}\left[\delta_{m'm+1}\sqrt{(j-m)(j+m+1)} - \delta_{m'm-1}\sqrt{(j+m)(j-m+1)}\right]\delta_{n'n}$$

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_3 \middle| {J \atop m,n} \right\rangle = D^J_{m',m}(\mathbf{J}_3)\delta_{n'n} = \delta_{m'm} m\ \delta_{n'n}$$

BOD matrix elements are the same after switching *m's* into *n's*
and changing sign of $\mathbf{J}_2$ matrix (*-conjugation)

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_{\bar{1}} \middle| {J \atop m,n} \right\rangle = \delta_{m'm} D^{J*}_{n',n}(\mathbf{J}_{\bar{1}}) = \tfrac{1}{2}\ \delta_{m'm}\left[\sqrt{(j-n)(j+n+1)}\delta_{n'n+1} + \sqrt{(j+n)(j-n+1)}\right]\delta_{n'n-1}]$$

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_{\bar{2}} \middle| {J \atop m,n} \right\rangle = \delta_{m'm} D^{J*}_{n',n}(\mathbf{J}_{\bar{2}}) = \tfrac{+i}{2}\ \delta_{m'm}\left[\sqrt{(j-n)(j+n+1)}\delta_{n'n+1} - \sqrt{(j+n)(j-n+1)}\right]\delta_{n'n-1}]$$

$$\left\langle {J \atop m',n'} \middle| \mathbf{J}_{\bar{3}} \middle| {J \atop m,n} \right\rangle = \delta_{m'm} D^{J*}_{n',n}(\mathbf{J}_{\bar{3}}) = \delta_{m'm} n\ \delta_{n'n}$$

Hamiltonian matrices for asymmetric rotor Hamiltonian

$$\mathbf{H} = \frac{1}{2}\left(\frac{\mathbf{J}_{\bar{1}}^2}{I_{\bar{1}}} + \frac{\mathbf{J}_{\bar{2}}^2}{I_{\bar{2}}} + \frac{\mathbf{J}_{\bar{3}}^2}{I_{\bar{3}}}\right) = A\mathbf{J}_{\bar{1}}^2 + B\mathbf{J}_{\bar{2}}^2 + C\mathbf{J}_{\bar{3}}^2$$

First are matrix formulas for BOD J^2 components.

$$\mathbf{J}_{\bar{1}}^2 \left|{J \atop m,n}\right\rangle = \frac{1}{2}\sqrt{(j-n)(j+n+1)}\,\mathbf{J}_{\bar{1}}\left|{J \atop m,n+1}\right\rangle + \frac{1}{2}\sqrt{(j+n)(j-n+1)}\,\mathbf{J}_{\bar{1}}\left|{J \atop m,n-1}\right\rangle$$

$$= \frac{1}{4}\sqrt{(j-n)(j+n+1)}\sqrt{(j-n-1)(j+n+2)}\left|{J \atop m,n+2}\right\rangle + \frac{1}{4}(j-n)(j+n+1)\left|{J \atop m,n}\right\rangle + \frac{1}{4}\sqrt{(j+n)(j-n+1)}\sqrt{(j+n-1)(j-n+2)}\left|{J \atop m,n-2}\right\rangle + \frac{1}{4}(j+n)(j-n+1)\left|{J \atop m,n}\right\rangle$$

$$= \frac{\sqrt{(j-n)(j-n-1)(j+n+1)(j+n+2)}}{4}\left|{J \atop m,n+2}\right\rangle + \frac{j(j+1)-n^2}{2}\left|{J \atop m,n}\right\rangle + \frac{\sqrt{(j+n)(j+n-1)(j-n+1)(j-n+2)}}{4}\left|{J \atop m,n-2}\right\rangle$$

$$\mathbf{J}_{\bar{2}}^2 \left|{J \atop m,n}\right\rangle = \frac{i}{2}\sqrt{(j-n)(j+n+1)}\,\mathbf{J}_{\bar{2}}\left|{J \atop m,n+1}\right\rangle - \frac{i}{2}\sqrt{(j+n)(j-n+1)}\,\mathbf{J}_{\bar{2}}\left|{J \atop m,n-1}\right\rangle$$

$$= \frac{-1}{4}\sqrt{(j-n)(j+n+1)}\sqrt{(j-n-1)(j+n+2)}\left|{J \atop m,n+2}\right\rangle + \frac{1}{4}(j-n)(j+n+1)\left|{J \atop m,n}\right\rangle \frac{-1}{4}\sqrt{(j+n)(j-n+1)}\sqrt{(j+n-1)(j-n+2)}\left|{J \atop m,n-2}\right\rangle + \frac{1}{4}(j+n)(j-n+1)\left|{J \atop m,n}\right\rangle$$

$$= -\frac{\sqrt{(j-n)(j-n-1)(j+n+1)(j+n+2)}}{4}\left|{J \atop m,n+2}\right\rangle + \frac{j(j+1)-n^2}{2}\left|{J \atop m,n}\right\rangle - \frac{\sqrt{(j+n)(j+n-1)(j-n+1)(j-n+2)}}{4}\left|{J \atop m,n-2}\right\rangle$$

$$\mathbf{J}_{\bar{3}}^2 \left|{J \atop m,n}\right\rangle = n^2\left|{J \atop m,n}\right\rangle$$

This gives the rigid asymmetric-top matrix formula for general *A, B, C* and *J*.:

$$(A\mathbf{J}_{\bar{1}}^2 + B\mathbf{J}_{\bar{2}}^2 + C\mathbf{J}_{\bar{3}}^2)\left|{J \atop m,n}\right\rangle =$$

$$= (A-B)\frac{\sqrt{(j-n)(j-n-1)(j+n+1)(j+n+2)}}{4}\left|{J \atop m,n+2}\right\rangle + \left[(A+B)\frac{j(j+1)-n^2}{2} + Cn^2\right]\left|{J \atop m,n}\right\rangle + (A-B)\frac{\sqrt{(j+n)(j+n-1)(j-n+1)(j-n+2)}}{4}\left|{J \atop m,n-2}\right\rangle$$

(*J=1*)-Matrix for *A=1*, *B=2*, *C=3*.

$$\left\langle {}^{1}_{m,n'} \middle| \mathbf{J}_{\bar{1}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} \cdot & \frac{\sqrt{2}}{2} & \cdot \\ \frac{\sqrt{2}}{2} & \cdot & \frac{\sqrt{2}}{2} \\ \cdot & \frac{\sqrt{2}}{2} & \cdot \end{pmatrix}, \quad \left\langle {}^{1}_{m,n'} \middle| \mathbf{J}_{\bar{2}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} \cdot & \frac{i\sqrt{2}}{2} & \cdot \\ \frac{-i\sqrt{2}}{2} & \cdot & \frac{i\sqrt{2}}{2} \\ \cdot & \frac{-i\sqrt{2}}{2} & \cdot \end{pmatrix}, \quad \left\langle {}^{1}_{m,n'} \middle| \mathbf{J}_{\bar{3}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$$\left\langle {}^{1}_{m,n'} \middle| \mathbf{J}^2_{\bar{1}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} \frac{1}{2} & \cdot & \frac{1}{2} \\ \cdot & 1 & \cdot \\ \frac{1}{2} & \cdot & \frac{1}{2} \end{pmatrix}, \quad \left\langle {}^{1}_{m,n'} \middle| \mathbf{J}^2_{\bar{2}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} \frac{1}{2} & \cdot & -\frac{1}{2} \\ \cdot & 1 & \cdot \\ -\frac{1}{2} & \cdot & \frac{1}{2} \end{pmatrix}, \quad \left\langle {}^{1}_{m,n'} \middle| \mathbf{J}^2_{\bar{3}} \middle| {}^{1}_{m,n} \right\rangle = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & 0 & \cdot \\ \cdot & \cdot & +1 \end{pmatrix}.$$

$$\left\langle A\mathbf{J}^2_{\bar{1}} + B\mathbf{J}^2_{\bar{2}} + C\mathbf{J}^2_{\bar{3}} \right\rangle^{J=1} = \begin{pmatrix} \frac{A}{2}+\frac{B}{2}+C & \cdot & \frac{A}{2}-\frac{B}{2} \\ \cdot & A+B & \cdot \\ \frac{A}{2}-\frac{B}{2} & \cdot & \frac{A}{2}+\frac{B}{2}+C \end{pmatrix} = \begin{pmatrix} \frac{1}{2}+\frac{2}{2}+3 & \cdot & \frac{1}{2}-\frac{2}{2} \\ \cdot & 1+2 & \cdot \\ \frac{1}{2}-\frac{2}{2} & \cdot & \frac{1}{2}+\frac{2}{2}+3 \end{pmatrix} = \begin{pmatrix} \frac{9}{2} & \cdot & -\frac{1}{2} \\ \cdot & 3 & \cdot \\ -\frac{1}{2} & \cdot & \frac{9}{2} \end{pmatrix}$$

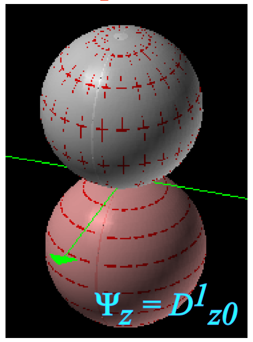
eigen-values: $(B+C=5, \quad A+B=3, \quad A+C=4)$

eigen-vectors: $\begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ -1/\sqrt{2} & 0 & +1/\sqrt{2} \end{pmatrix}$

$\left|B+C\right\rangle = 1/\sqrt{2}\left|{}^{1}_{m,+1}\right\rangle \quad -1/\sqrt{2}\left|{}^{1}_{m,-1}\right\rangle$ *y-like*

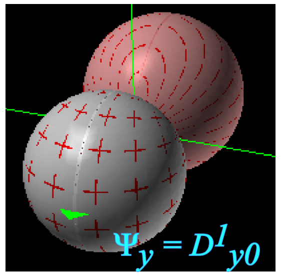
$\left|A+B\right\rangle = \quad +\left|{}^{1}_{m,0}\right\rangle$ *z-like*

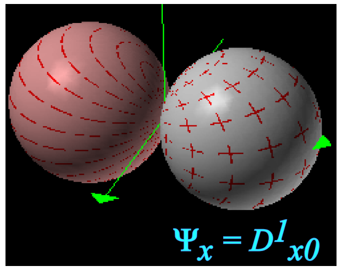
$\left|A+C\right\rangle = 1/\sqrt{2}\left|{}^{1}_{m,+1}\right\rangle \quad +1/\sqrt{2}\left|{}^{1}_{m,-1}\right\rangle$ *x-like*



j = 1
Standing
p-Waves

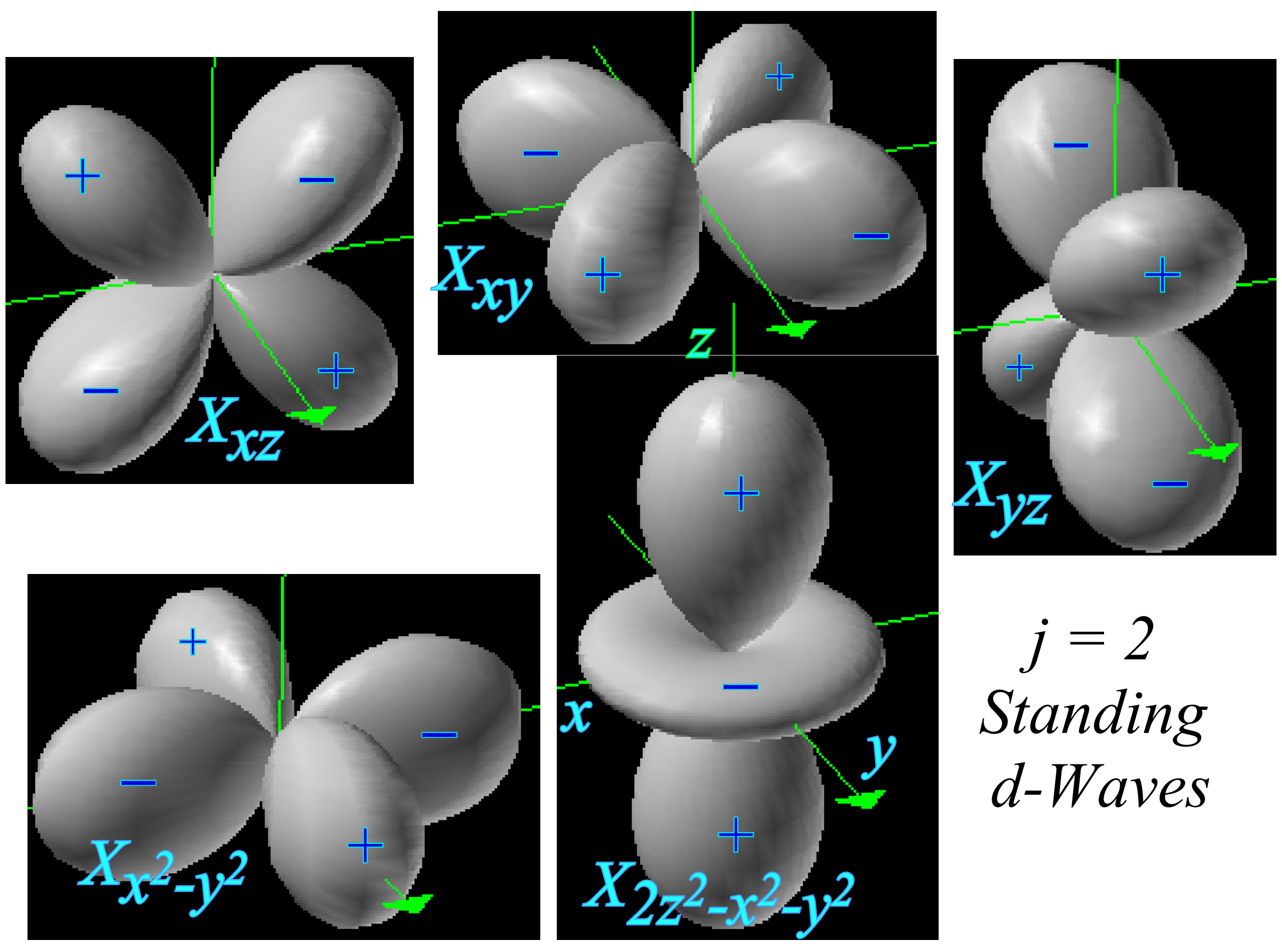
Body-based J=1
vector-like eigenfunctions





(*J*=2)-Matrix for *A*=*1*, *B*=*2*, *C*=*3*.

$$\left\langle A\mathbf{J}_{\bar{1}}^2 + B\mathbf{J}_{\bar{2}}^2 + C\mathbf{J}_{\bar{3}}^2 \right\rangle^{J=2} = \begin{pmatrix} (A+B)+4C & \cdot & \frac{\sqrt{6}}{2}(A-B) & \cdot & \cdot \\ \cdot & \frac{5}{2}(A+B)+C & \cdot & \frac{3}{2}(A-B) & \cdot \\ \frac{\sqrt{6}}{2}(A-B) & \cdot & 3(A+B) & \cdot & \frac{\sqrt{6}}{2}(A-B) \\ \cdot & \frac{3}{2}(A-B) & \cdot & \frac{5}{2}(A+B)+C & \cdot \\ \cdot & \cdot & \frac{\sqrt{6}}{2}(A-B) & \cdot & (A+B)+4C \end{pmatrix} = \begin{pmatrix} 15 & & -\frac{\sqrt{6}}{2} & & \\ & \frac{15}{2} & & \frac{-3}{2} & \\ -\frac{\sqrt{6}}{2} & & 6 & & -\frac{\sqrt{6}}{2} \\ & \frac{-3}{2} & & \frac{15}{2} & \\ & & -\frac{\sqrt{6}}{2} & & 15 \end{pmatrix}$$



j = 2
Standing
d-Waves

$(J=2)$-Matrix for $A=1$, $B=2$, $C=3$.

$$\left\langle A\mathbf{J}_1^2 + B\mathbf{J}_2^2 + C\mathbf{J}_3^2 \right\rangle^{J=2} = \begin{pmatrix} (A+B)+4C & \cdot & \frac{\sqrt{6}}{2}(A-B) & \cdot & \cdot \\ \cdot & \frac{5}{2}(A+B)+C & \cdot & \frac{3}{2}(A-B) & \cdot \\ \frac{\sqrt{6}}{2}(A-B) & \cdot & 3(A+B) & \cdot & \frac{\sqrt{6}}{2}(A-B) \\ \cdot & \frac{3}{2}(A-B) & \cdot & \frac{5}{2}(A+B)+C & \cdot \\ \cdot & \cdot & \frac{\sqrt{6}}{2}(A-B) & \cdot & (A+B)+4C \end{pmatrix} = \begin{pmatrix} 15 & & -\frac{\sqrt{6}}{2} & & \\ & \frac{15}{2} & & \frac{-3}{2} & \\ -\frac{\sqrt{6}}{2} & & 6 & & -\frac{\sqrt{6}}{2} \\ & \frac{-3}{2} & & \frac{15}{2} & \\ & & -\frac{\sqrt{6}}{2} & & 15 \end{pmatrix}$$

Matrix is nearly diagonalized in standing-wave D_2-symmetry basis

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle, \quad \left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle, \quad \left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle$$

$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle, \quad \left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

The following basis transformation "almost diagonalizes" $\langle \mathbf{H} \rangle^{J=2}$ by reducing it to block form.
Let: $\Sigma = A+B$ and $\Delta = A-B$ to shorten expressions.

$$\left(\tfrac{1}{\sqrt{2}}\right)\begin{pmatrix} 1 & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & -1 \\ \cdot & 1 & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & -1 & \cdot \\ \cdot & \cdot & \sqrt{2} & \cdot & \cdot \end{pmatrix} \begin{pmatrix} 4C-\Sigma & \cdot & \frac{\sqrt{6}\Delta}{2} & \cdot & \cdot \\ \cdot & C+\frac{\Sigma}{2} & \cdot & \frac{3\Delta}{2} & \cdot \\ \frac{\sqrt{6}\Delta}{2} & \cdot & \Sigma & \cdot & \frac{\sqrt{6}\Delta}{2} \\ \cdot & \frac{3\Delta}{2} & \cdot & C+\frac{\Sigma}{2} & \cdot \\ \cdot & \cdot & \frac{\sqrt{6}\Delta}{2} & \cdot & 4C-\Sigma \end{pmatrix} \begin{pmatrix} 1 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \sqrt{2} \\ \cdot & \cdot & 1 & -1 & \cdot \\ 1 & -1 & \cdot & \cdot & \cdot \end{pmatrix} \left(\tfrac{1}{\sqrt{2}}\right) + 2\Sigma\mathbf{1}$$

$$= \begin{pmatrix} 4C+\Sigma & \cdot & \cdot & \cdot & \sqrt{3}\Delta \\ \cdot & 4C+\Sigma & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+\frac{5\Sigma}{2}+\frac{3\Delta}{2} & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+\frac{5\Sigma}{2}-\frac{3\Delta}{2} & \cdot \\ \sqrt{3}\Delta & \cdot & \cdot & \cdot & 3\Sigma \end{pmatrix} = \begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

New D_2 basis:

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$
$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$
$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$
$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$
$$\left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle$$

Completing diagonalization from new D_2 basis:

$$\begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

$$\left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle$$

D_2	**1**	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
A_1	1	1	1	1
A_2	1	-1	1	−1
B_1	1	1	-1	−1
B_2	1	-1	-1	1

C_2^x	**1**	$\mathbf{R}_x$
+	1	1
−	1	−1

×

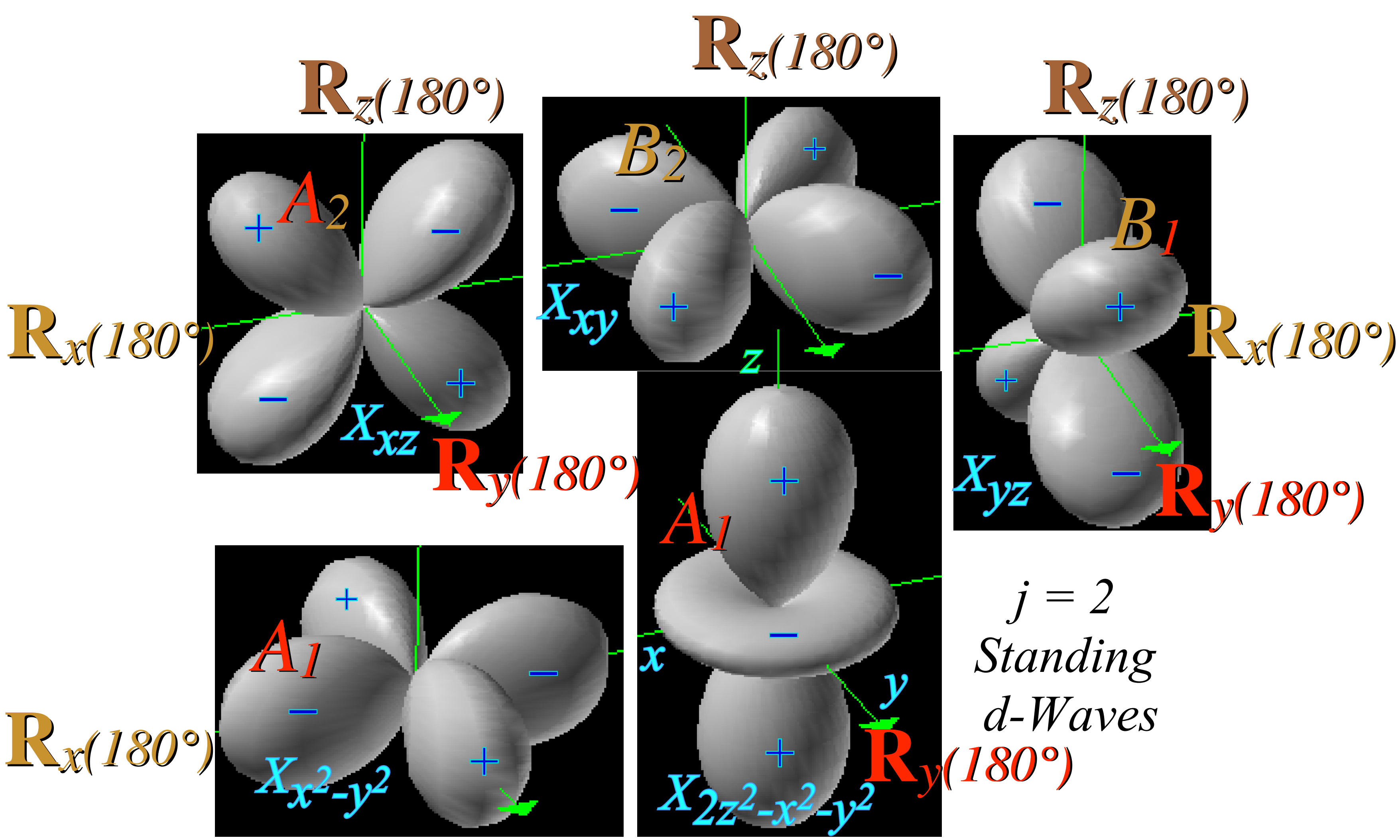
C_2^y	**1**	$\mathbf{R}_y$
+	1	1
−	1	−1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	**1**	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$+\cdot+=A_1$	1	1	1	1
$-\cdot+=A_2$	1	-1	1	−1
$+\cdot-=B_1$	1	1	-1	−1
$-\cdot-=B_2$	1	-1	-1	1



Completing diagonalization from new D_2 basis:

$$\begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

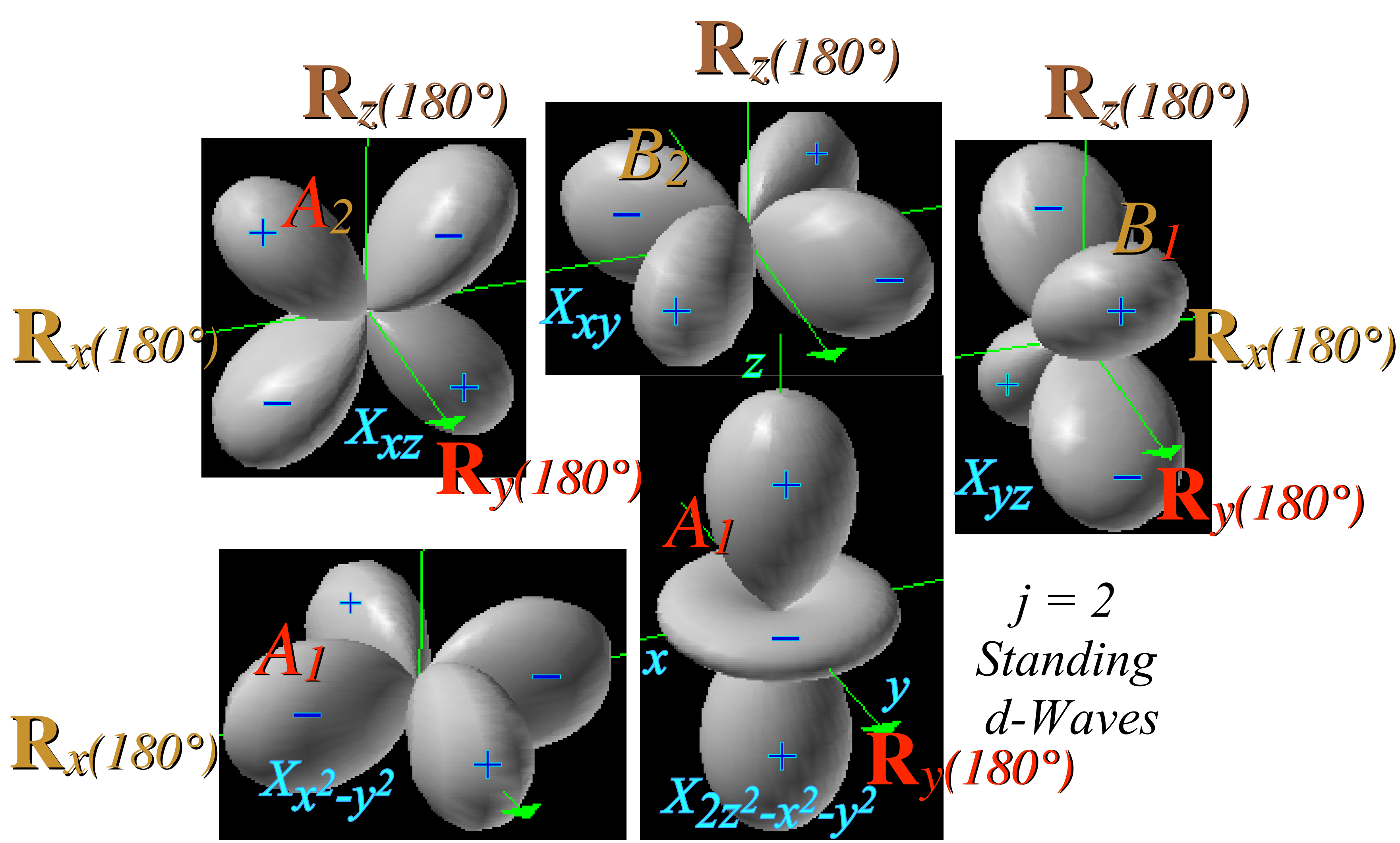
$$\left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle$$

Need only diagonalize the two A_1's:

(It is n=0 versus n=2+)

$$\begin{pmatrix} 4C+A+B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & 3A+3B \end{pmatrix} \quad \begin{matrix} \left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle \\ \left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle \end{matrix}$$

D_2	**1**	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
A_1	1	1	1	1
A_2	1	-1	1	−1
B_1	1	1	-1	−1
B_2	1	-1	-1	1



j = 2
Standing
d-Waves

Completing diagonalization from new D_2 basis:

$$\begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle$$
$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle - \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle$$
$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +1}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -1}\right\rangle$$
$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +1}\right\rangle - \tfrac{1}{\sqrt{2}}\left|{2 \atop -1}\right\rangle$$
$$\left|A_1 0\right\rangle = \left|{2 \atop 0}\right\rangle$$

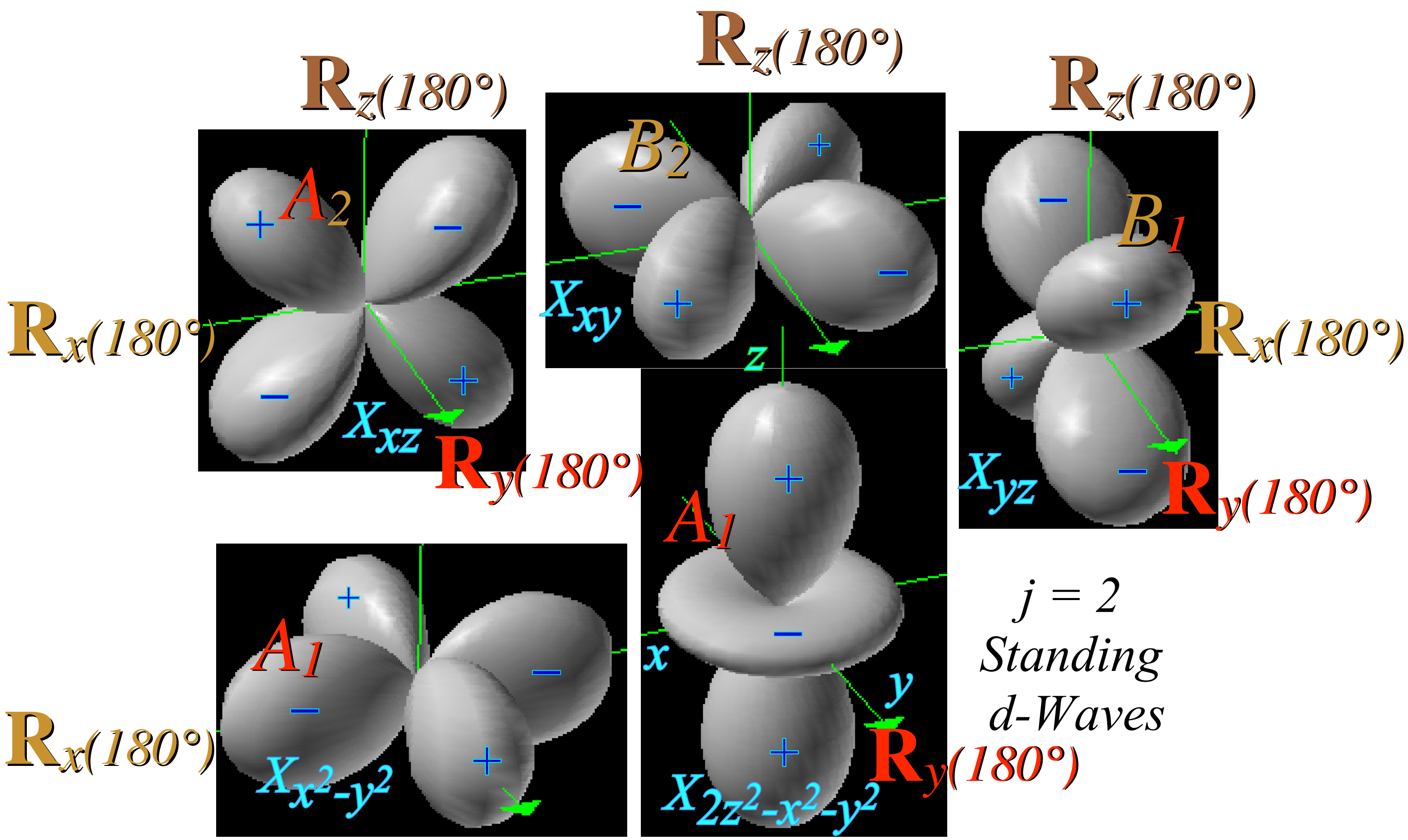
Need only diagonalize the two A_1's:

(It is n=0 versus n=2⁺)

$$\begin{pmatrix} 4C+A+B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & 3A+3B \end{pmatrix} \begin{matrix} \left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle \\ \left|A_1 0\right\rangle = \left|{2 \atop 0}\right\rangle \end{matrix}$$

$$= (2C+2A+2B)\cdot\mathbf{1} + \begin{pmatrix} 2C-A-B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & -(2C-A-B) \end{pmatrix}$$

D_2	**1**	**R_x**	**R_y**	**R_z**
A_1	1	1	1	1
A_2	1	-1	1	−1
B_1	1	1	-1	−1
B_2	1	-1	-1	1



Completing diagonalization from new D_2 basis:

$$\begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle$$

$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+1\end{smallmatrix}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-1\end{smallmatrix}\right\rangle$$

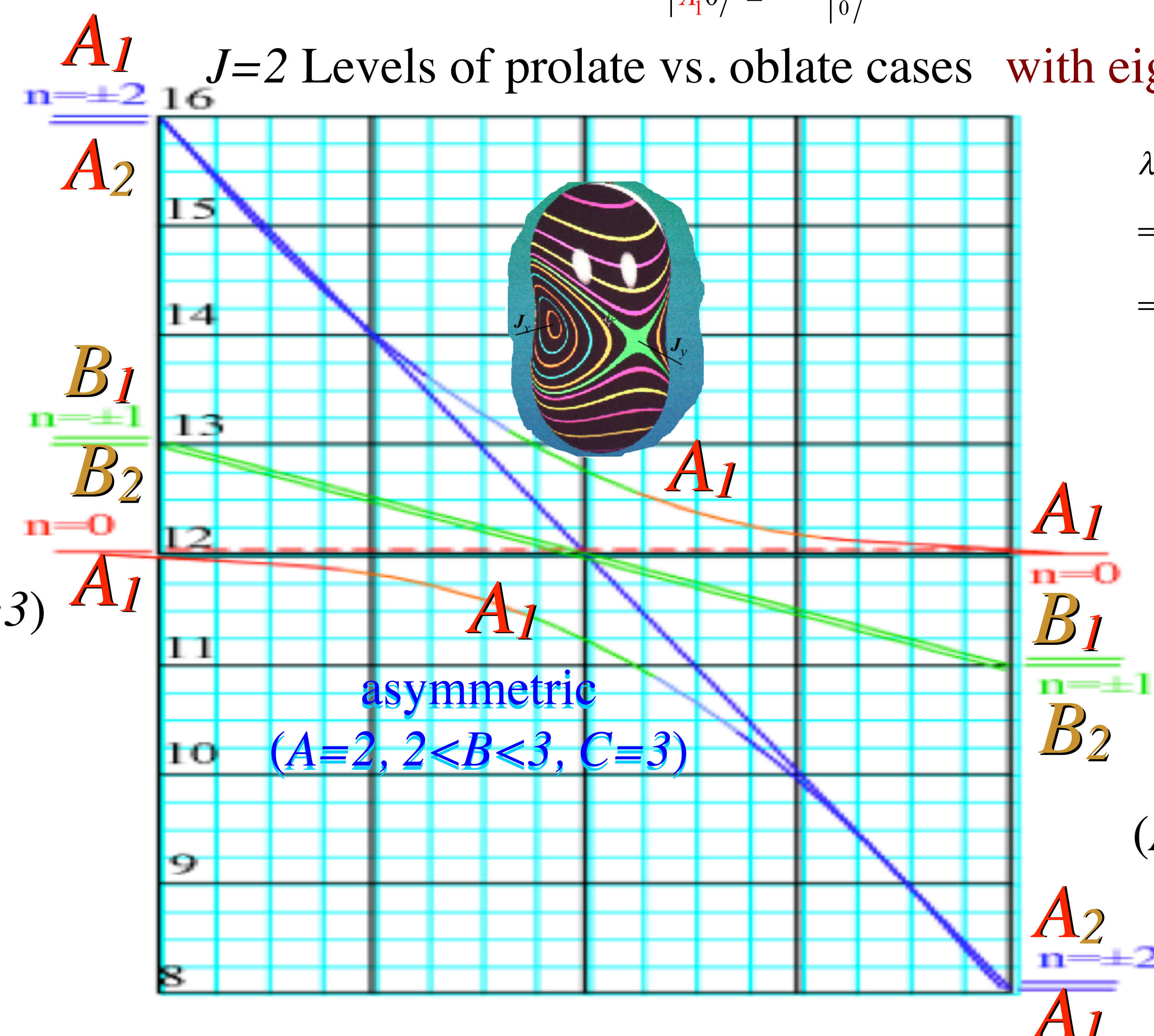
$$\left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle$$

Need only diagonalize the two A_1's:

(It is n=0 versus n=2+)

$$\begin{pmatrix} 4C+A+B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & 3A+3B \end{pmatrix} \begin{matrix} \left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\+2\end{smallmatrix}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\begin{smallmatrix}2\\-2\end{smallmatrix}\right\rangle \\ \left|A_1 0\right\rangle = \left|\begin{smallmatrix}2\\0\end{smallmatrix}\right\rangle \end{matrix}$$

$$= (2C+2A+2B)\cdot\mathbf{1} + \begin{pmatrix} 2C-A-B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & -(2C-A-B) \end{pmatrix}$$



with eigenvalues:

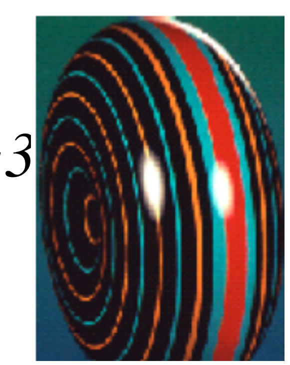
$$\lambda_{\pm} = 2C+2A+2B \pm \sqrt{(2C-A-B)^2 + 3(A-B)^2}$$

$$= 2(A+B+C) \pm 2\sqrt{C^2 - (A+B)C + A^2 - AB + B^2}$$

$$= 2C+4B \pm 2(C-B) = \begin{cases} 4C+2B \\ 6B \end{cases} \quad \text{if: } A=B$$

prolate
($A=2$, $B=2$, $C=3$)

oblate
($A=2$, $B=3$, $C=3$



A=B prolate case: ($A=2$, $B=2$, $C=3$)

$B(J(J+1) + (C-B)n^2 = 2B+4C = 4+12 = 16$ ($n=\pm 2$)

$5B+C = 10+3 = 13$ ($n=\pm 1$) , $6B = 12$ ($n=0$)

B=C oblate case: ($A=1$, $B=2$, $C=2$)

$B(J(J+1) + (A-B)n^2 = 2B+4A = 4+4 = 8$ ($n=\pm 2$)

$5B+A = 10+1 = 11$ ($n=\pm 1$) , $6B = 12$ ($n=0$)

Completing diagonalization from new D_2 basis:

$$\begin{pmatrix} 4C+A+B & \cdot & \cdot & \cdot & \sqrt{3}(A-B) \\ \cdot & 4C+A+B & \cdot & \cdot & \cdot \\ \cdot & \cdot & C+4A+B & \cdot & \cdot \\ \cdot & \cdot & \cdot & C+A+4B & \cdot \\ \sqrt{3}(A-B) & \cdot & \cdot & \cdot & 3A+3B \end{pmatrix}$$

$$\left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle$$
$$\left|B_2 2^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle - \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle$$
$$\left|B_1 1^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +1}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -1}\right\rangle$$
$$\left|A_2 1^-\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +1}\right\rangle - \tfrac{1}{\sqrt{2}}\left|{2 \atop -1}\right\rangle$$
$$\left|A_1 0\right\rangle = \left|{2 \atop 0}\right\rangle$$

Need only diagonalize the two A_1's:

(It is n=0 versus n=2+)

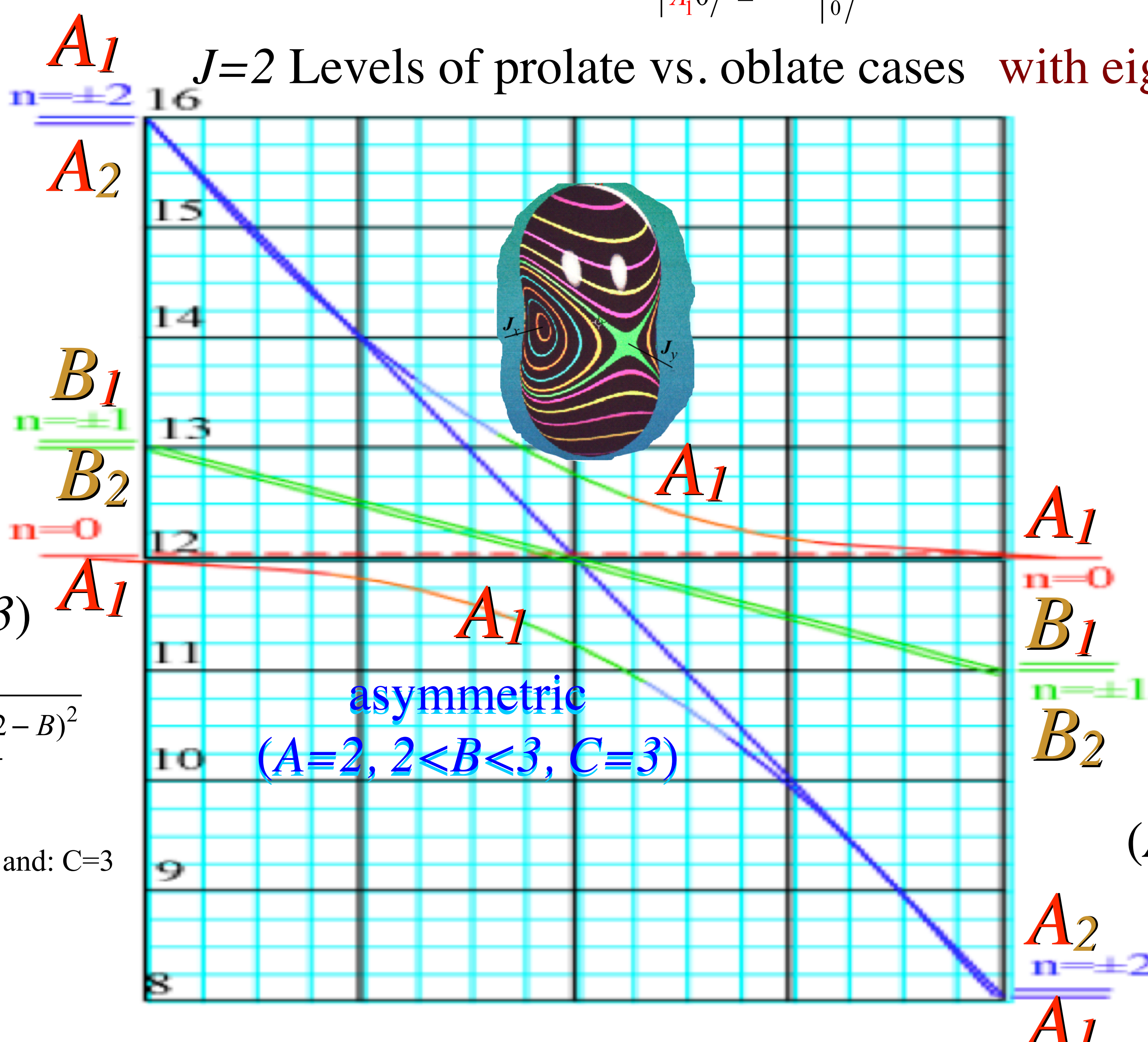
$$\begin{pmatrix} 4C+A+B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & 3A+3B \end{pmatrix} \quad \left|A_1 2^+\right\rangle = \tfrac{1}{\sqrt{2}}\left|{2 \atop +2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|{2 \atop -2}\right\rangle, \quad \left|A_1 0\right\rangle = \left|{2 \atop 0}\right\rangle$$

$$= (2C+2A+2B)\cdot\mathbf{1} + \begin{pmatrix} 2C-A-B & \sqrt{3}(A-B) \\ \sqrt{3}(A-B) & -(2C-A-B) \end{pmatrix}$$

with eigenvalues:

$$\begin{pmatrix} 14+B & \sqrt{3}(2-B) \\ \sqrt{3}(2-B) & 6+3B \end{pmatrix} =$$

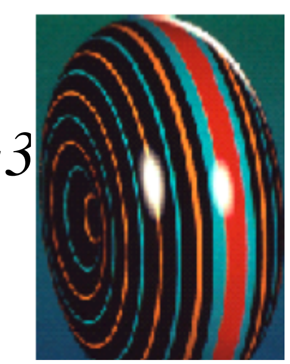
$$(10+2B)\cdot\mathbf{1} + \begin{pmatrix} 4-B & \sqrt{3}(2-B) \\ \sqrt{3}(2-B) & -(4-B) \end{pmatrix}$$



prolate
(*A*=2, *B*=2, *C*=3)

$$\lambda_\pm = 10+2B \pm \sqrt{(4-B)^2 + 3(2-B)^2}$$
$$= 2(5+B) \pm 2\sqrt{7-5B+B^2}$$
$$= 14 \pm 2 = \begin{cases} 16 \\ 12 \end{cases} \text{ if: } A=B=2 \text{ and: } C=3$$

oblate
(*A*=2, *B*=3, *C*=3



A=B prolate case: (*A*=2, *B*=2, *C*=3)

$B(J(J+1) + (C-B)n^2 = 2B+4C = 4+12 = 16$ ($n=\pm 2$)

$5B+C = 10+3 = 13$ ($n=\pm 1$) , $6B = 12$ ($n=0$)

B=C oblate case: (*A*=1, *B*=2, *C*=2)

$B(J(J+1) + (A-B)n^2 = 2B+4A = 4+4 = 8$ ($n=\pm 2$)

$5B+A = 10+1 = 11$ ($n=\pm 1$) , $6B = 12$ ($n=0$)

New geometric approach to rotational eigenstates and spectra

Introduction to Rotational Energy Surfaces (RES)

Symmetric vs Asymmetry RES

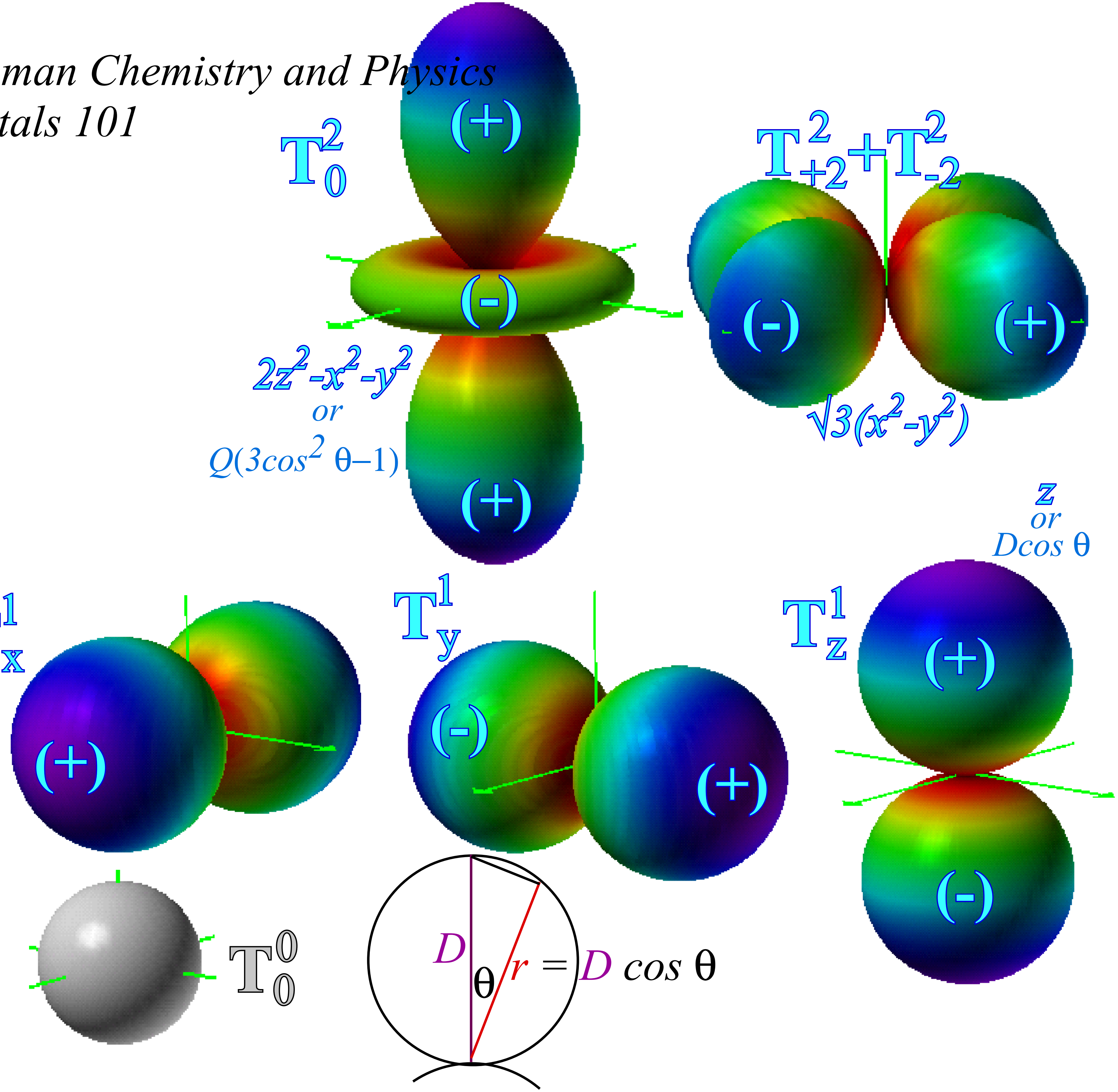
Spherical rotor RES

Review of freshman Chemistry and Physics
Electronic orbitals 101

Quadrupoles
(d-orbitals)

Dipoles
(p-orbitals)

Monopole
(s-orbital)



Review of freshman Chemistry and Physics (contd)

Momentum 101 $p = m\,v$ *(linear)* $J = L = I\,\omega$ *(rotation)* BANG!

Energy 101 $E = \frac{1}{2} m\,v^2 = p^2/2m$ $E = \frac{1}{2} I\,\omega^2 = J^2/2I$ $BUCK$

Simple Rigid Rotor Hamiltonian... (Hamiltonian H=E is energy [$BUCK$] in terms of momentum [BANG!])

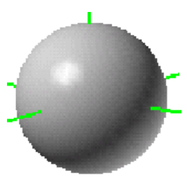
$$\mathbf{H} = A\mathbf{J}_x^2 + B\mathbf{J}_y^2 + C\mathbf{J}_z^2 + \cdots$$

...and its multi-pole expansion...

$$\left(\frac{A+B+C}{3}\right)\left(\mathbf{J}_x^2 + \mathbf{J}_y^2 + \mathbf{J}_z^2\right) + \left(\frac{2C-A-B}{6}\right)\left(2\mathbf{J}_z^2 - \mathbf{J}_x^2 - \mathbf{J}_y^2\right) + \left(\frac{A-B}{2}\right)\left(\mathbf{J}_x^2 - \mathbf{J}_y^2\right)$$

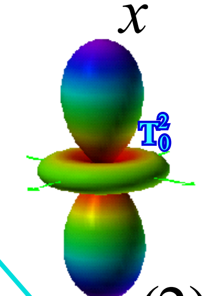
Spherical Top *(A=B=C)*

$\mathbf{H} = B\,\mathbf{J}^2$



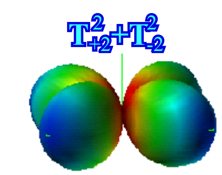
$$\mathbf{T}_0^{(0)} = \mathbf{J}^2$$

Symmetric Top *(A=B≠C)*



$$2\mathbf{T}_0^{(2)}$$

$\mathbf{H} = B\,\mathbf{J}^2 + (C - B)(2/3)\mathbf{T}_0^{(2)}$



$$\sqrt{\frac{2}{3}}\left(\mathbf{T}_2^{(2)} + \mathbf{T}_{-2}^{(2)}\right)$$

Asymmetric Top *(A≠B≠C)*

$$\mathbf{H} = B\,\mathbf{J}^2 + (2C - A - B)/3\;\mathbf{T}_0^{(2)} + (A - B)/\sqrt{6}\left(\mathbf{T}_2^{(2)} + \mathbf{T}_{-2}^{(2)}\right)$$

(Derivation follows next lecture…)

As of April 3, 2014

Links to the current Harter-Soft LearnIt web apps for Physics

Bold links have default redirect pages. *Italics* are not yet meant for production.Red: the final stages of testing.

List of *production* Harter-Soft Web Apps & Textbooks (For public)

Classical Mechanics with a Bang! - URL is "http://www.uark.edu/ua/modphys/markup/CMwBangWeb.html"
Quantum Theory for the Computer Age - URL is "http://www.uark.edu/ua/modphys/markup/QTCAWeb.html"
LearnIt Web Applications - URL is "http://www.uark.edu/ua/modphys/markup/LearnItWeb.html"

Individual web-apps for current classes:

BohrIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BohrItWeb.html"
BounceIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BounceItWeb.html"
BoxIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/BoxItWeb.html"
CoulIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/CoulItWeb.html"
Cycloidulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/CycloidulumWeb.html"
JerkIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/JerkItWeb.html"
MolVibes - Production; URL is "http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html"
Pendulum - Production; URL is "http://www.uark.edu/ua/modphys/markup/PendulumWeb.html"
QuantIt - Production; URL is "http://www.uark.edu/ua/modphys/markup/QuantItWeb.html"

The old relativity website (2005):
Relativity - Pirelli Entrant - Production; URL is "**http://www.uark.edu/ua/pirelli**" or "http://www.uark.edu/ua/pirelli/html/default.html"

Newer relativity web-apps currently being developed (2013-)
RelativIt Production; URL is "http://www.uark.edu/ua/modphys/markup/RelativItWeb.html"
RelaWavity Production; URL is "http://www.uark.edu/ua/modphys/markup/RelaWavityWeb.html"

Additional classical wep-apps:
Trebuchet Production; URL is "http://www.uark.edu/ua/modphys/markup/TrebuchetWeb.html"
WaveIt Production; URL is "http://www.uark.edu/ua/modphys/markup/WaveItWeb.html"

Link to master list of all Harter-Soft Web Apps & Textbooks (Prod, Testing, & Developement)

http://www.uark.edu/ua/modphys/testing/markup/Harter-SoftWebApps.html